NAT'L INST. OF STAND & TECH
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A11103 066665

NBS SPECIAL PUBLICATION 513

U.S. DEPARTMENT OF COMMERCE / National Bureau of Standards

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Reaction Rate and Photochemical Data for Atmospheric Chemistry - 1977

Special publication no. 513

Edited by

Robert F. Hampson, Jr. and David Garvin

National Measurement Laboratory
National Bureau of Standards
Washington, D.C. 20234

Sponsored by the
Department of Transportation
National Aeronautics & Space Administration
Office of Standard Reference Data, NBS
Office of Environmental Measurements, NBS

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NATIONAL BUREAU OF STANDARDS, Ernest Ambler, Director

Issued May 1978

Library of Congress Cataloging in Publication Data

Main entry under title:

Reaction rate and photochemical data for atmospheric chemistry, 1977.

(National Bureau of Standards special publication ; 513)

Supt. of Docs. no.: C13.10:513

1. Atmospheric chemistry--Tables. 2. Chemical reaction, Rate of--Tables, etc. 3. Photochemistry--Tables. I. Hampson, Robert F. II. Garvin, David, 1923- III. United States. Dept. of Transportation IV. United States. National Bureau of Standards. V. Series: United States. National Bureau of Standards. Special publication ; 513.

QC100.U57 no. 513 [QC879.6] 602'.1s [551.5'11] 78-606033

National Bureau of Standards Special Publication 513

Nat. Bur. Stand. (U.S.) Spec. Publ. 513, 111 pages (May 1978)

CODEN: XNBSAV

U.S. GOVERNMENT PRINTING OFFICE

WASHINGTON: 1978

For sale by the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402

Stock No. 003-003-01924-1 Price $2.75

(Add 25 percent additional for other than U.S. mailing).

FOREWORD

The National Standard Reference Data System was established in 1963 for the purpose of promoting the critical evaluation and dissemination of numerical data of the physical sciences. The program is coordinated by the Office of Standard Reference Data of the National Bureau of Standards, but involves the efforts of many groups in universities, government laboratories, and private industry. The primary aim of the program is to provide compilations of critically evaluated numerical data. These tables are published in the Journal of Physical and Chemical Reference Data, The NSRDS-NBS Publication Series of the National Bureau of Standards, and through other appropriate channels.

The present report consists of tables of data assembled for use in modelling the chemistry of the stratosphere. It represents contributions from the Chemical Kinetics Information Center, other NSRDS data centers, and a number of individual experts. Support for the preparation of those tables has been provided by the Department of Transportation under the High Altitude Pollution Program, by the National Aeronautics and Space Administration under the Upper Atmosphere Research Program, and by the Office of Standard Reference Data, N.B.S. and the Office of Environmental Measurements, N.B.S.

David R. Lide, Jr.
Chief, Office of Standard
Reference Data

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Reaction Rate and Photochemical Data for Atmospheric Chemistry - 1977*

R. F. Hampson, D. Garvin, Editors

A table of data for gas phase chemical reactions and photochemistry of neutral species is presented. Specifically, it gives preferred values for reaction rate constants, photoabsorption cross sections, and quantum yields of primary photochemical processes and also cites recent experimental work (to December 1977). It is intended to provide the basic physical chemical data needed as input data for calculations modelling atmospheric chemistry. An auxiliary table of thermochemical data for the pertinent chemical species is given in the appendix.

Key words: Air pollution; atmospheric chemistry; chemical kinetics; data evaluation; gas phase; photoabsorption cross section; photochemistry; quantum yield; rate constant.

1. Introduction

This technical note consists of a table of data on the kinetics of chemical reactions and the photochemistry of neutral species. It is designed for use in modelling the chemistry of the stratosphere and, to a more limited extent, the polluted troposphere and also the interpretation of laboratory experiments. The table of rate and photochemical data is supplemented by a table of thermochemical data for the species involved.

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*This work was supported by the High Altitude Pollution Program of the Federal Aviation Administration, U. S. Department of Transportation, by the Upper Atmospheric Research Program of the National Aeronautics and Space Administration, and by the Office of Standard Reference Data, N.B.S. and the Office of Environmental Measurements, N.B.S.

Earlier versions of this table have been issued as D. Garvin (editor) "Chemical Kinetics Data Survey IV" NBSIR 73-203 (1973); D. Garvin and R. F. Hampson (editors) "Chemical Kinetics Data Survey VII" NBSIR 74-430 (1974); and R. F. Hampson and D. Garvin (editors) "Chemical Kinetic and Photochemical Data for Modelling Atmospheric Chemistry" NBS Technical Note 866 (1975). The table appearing in NBS Technical Note 866 was also published in the U. S. Department of Transportation's Climatic Impact Assessment Program Monograph 1 "The Natural Stratosphere of 1974" E. Reiter, editor (1975). The present table supersedes all earlier versions.

Since the publication of NBS Technical Note 866 in 1975, a major effort in the evaluation of rate and photochemical data was undertaken for the NASA chlorofluoromethane assessment by its Laboratory Measurements Committee of which the present editors were members. The recommendations of this committee covering 104 chemical reactions and 48 photochemical processes are given in NASA Reference Publication 1010 "Chlorofluoromethanes and the Stratosphere" R. D. Hudson, editor, August 1977. These recommendations have been accepted by the editors of this table and are given here as preferred values. These recommendations are indicated either by the entry [†*NASA(1977)eval] or by the symbols [†*] immediately preceding the author's name in the reference column. The first notation is used to indicate that the committee has synthesized a preferred value from a consideration of all data sets. The latter designation is used when the committee has accepted the results of a particular study or of an existing evaluation.

Recommended values also are given for reactions not considered by the NASA Laboratory Measurements Committee. Some of these are drawn from other modern rate data evaluations, and the sources are indicated in the table. Other recommendations have been prepared for this work.

Rate data evaluation is a small but growing branch of physical chemistry. There are more recommended rate constants than contained in this table, but it does contain most of those which are applicable to atmospheric chemistry. Evaluations and compilations of rate data and on-going programs in these areas have been described in the recent review paper "Evaluation and Compilation of Reaction Rate Data" by R. F. Hampson and D. Garvin, Journal of Physical Chemistry 81, 2317-2319 (1977). A current extensive listing of sources of evaluated rate data, NBS List of Publications 73 "Chemical Kinetics Tables, Data Evaluations and Bibliographies. A Guide to the Literature" is available on request from the NBS Chemical Kinetics Information Center.

Three sets of detailed data sheets have been published by us in the course of preparing these tables. They are R. F. Hampson (editor) "Survey of Photochemical and Rate Data for Twenty-eight Reactions of Interest in Atmospheric Chemistry" J. Phys. Chem. Ref. Data 2, 267 (1973);

R. F. Hampson (editor) "Chemical Kinetics Data Survey VI, NBSIR 73-207 (1973); and D. Garvin (editor) "Chemical Kinetics Data Survey V" NBSIR 73-206 (1973), all recommendations contained in them (and still pertinent) are summarized in the present table.

We have also accepted many recommendations made by R. T. Watson in "Rate Constants for Reactions of $C\ell O_x$ of Atmospheric Interest" J. Phys. Chem. Ref. Data 6, 871 (1977) and by D. L. Baulch, et al "Evaluated Kinetic Data for High Temperature Reactions" Volume 1 (1972), Volume 2 (1973) and Volume 3 (1976), Butterworth and Co., London.

In addition to recommendations on rate and photochemical data the table includes listings of current research results. These data listings serve several purposes. Some simply record measurements, usually limited in number, on reactions for which it is not yet practical to give recommended values. Others show the data upon which a new recommendation is based. Still others show what has been done on a reaction since its rate constant was last evaluated. These new data may support the recommendation or suggest the need for modifications in the future.

2. Guide to the Table

2.1 General

This table provides current (December 1977) information on reaction rate constants, quantum yields and absorption cross sections. For many reactions, preferred values are given. The reactions included in the table are summarized in the index of reactions given in section 3.

Most of the important stratospheric reactions are in the tables. A number of the less important ones and some related systems are included, often simply for comparison.

The following remarks summarize the content of the table. It lists 416 reactions and gives a preferred value of the rate constant for 194 reactions; 136 based on recent reviews and 58 based on recent (1975-1977) experimental work. New data entries (1975-1977) are given for 252 reactions, showing substantial activity in the study of gas kinetics.

The following principles have been used in the selection and presentation of data:

a. Where a preferred value is given for a rate constant or photochemical quantity, it is so indicated by an asterisk [*] placed ahead of the entry in the reference column.

b. As indicated earlier an asterisk preceded by a dagger symbol [†*] is used to indicate those preferred values that have been recommended by the NASA Laboratory Measurements Committee and published in NASA Reference Publication 1010 "Chlorofluoromethanes and the Stratosphere" R. D. Hudson, editor, August 1977.

c. Where there is a recent published evaluation of the data and there are no newer data, the evaluation is adopted and usually marked with an asterisk. The original data covered by the evaluation are not listed separately. However this latter rule has not been applied when the evaluation has appeared within the past year.

d. Where there is an evaluation but there are new data, both are listed and a preferred value is indicated (marked by an asterisk).

e. Where desirable, the available recent data sets are listed, and a selection is made or a preferred value is synthesized from them.

2.2 Uncertainty in Recommended Value of a Rate Constant

The uncertainty assigned here to the recommended value of a rate constant is given in the column "Notes and reliability of log k". This is an estimate by the evaluator of the absolute accuracy of the preferred value. It is a subjective judgment derived from intercomparison of data sets, consideration of related reactions studied with the same technique, estimates of how well the parameters could have been controlled, and comparison with theory. It means that in the evaluators judgment, the true value will lie within the indicated limits to a high level of confidence (90 to 95 percent).

Usually the uncertainty is indicated by the term D in the expression: $\log_{10} k = C \pm D$. This is equivalent to the statement that k is uncertain to a factor of F where $D = \log_{10} F$. The statement that k has the value k_o and is uncertain to a factor of F means that $k_o/F < k < k_o F$.

Other forms used to indicate reliability are the following:

$A < k < B$ means k lies in the range between A and B
$k < (>) B$ means B is an upper (lower) limit
$k \sim B$ means B is only a rough guide to value of k
$k = A \pm B$ alternative form for stating reliability limits

At times a rate constant expression is quoted from a paper with individual uncertainties for the rate parameters as $k = (A \pm a) \exp(-B \pm b/T)$. These measures are those provided by the author and often are indications of precision, not overall reliability.

Some notes are in order, regarding the statement of the uncertainty in the recommended value of the rate constant for those recommended values recommended by the NASA Laboratory Measurements Committee. Those recommendations were made for the limited temperature range 200-300 K. The uncertainty is indicated for T = 230 K, a typical midstratospheric temperature and in some cases allowance for extrapolation from higher temperatures was necessary. This is why occasionally the entry consists of the value of a rate constant measured at 298 K, the symbols [†*] immediately ahead of the entry in the reference column to show that this value has been adopted by the Committee for the temperature range 200-300 K, and a statement of the uncertainty in the preferred value at T = 230 K. This stated uncertainty will generally be larger than the uncertainty in the measured value (measured at 298 K) to allow for the additional uncertainty introduced by extrapolation to T = 230 K.

For the recommendations made by the NASA Laboratory Committee the indicated uncertainties in NASA Reference Publication 1010 have been doubled in the present table in order to make the reliability statement analogous to a "95 percent confidence level".

2.3 Conventions Concerning Rate Constants

a. General Convention. Almost all of the reactions in the table are elementary processes. For them the rate expression is derivable from a statement of the reaction, e.g.

$$A + 2B \rightarrow AB_2$$

$$-d[A]/dt = -(1/2)\, d[B]/dt = d[AB_2]/dt = k[A][B]^2$$

Note that the stoichiometric coefficient for B, i.e. 2, appears in the denominator before B's rate of change (which is equal to $2k[A][B]^2$) and as a power on the right hand side.

Wherever there may be any doubt an explicit rate expression is given.

b. Dissociation and Combination Reactions. Some reactions of these types are not of integral kinetic order over the stratospheric pressure and temperature range. That is, although they require an energy transfer agent, "M," they are in the "pressure fall-off region". For some such reactions we tabulate rate constants that include the effect of the energy transfer agent and give rates for various altitudes. The reactions are written to demphasize "M," e.g.,

$$NO_2 + NO_3 \ (+M) \rightarrow N_2O_5 \ (+M)$$

$$HNO_3 \xrightarrow{M} HO + NO_2$$

The rate expressions to be used do not have the concentration of M in them, e.g., Rate = $k[NO_2]\ [NO_3]$ and $k[HNO_3]$ respectively. The units given for the k's, s^{-1} for first order, and cm^{+3} molecule$^{-1}s^{-1}$ for second order, are consistent with this convention.

The altitude, temperature and number density regime used in these cases is

altitude/km	temp./K	log[M]/molecule cm^{-3}
15	217	18.60
20	217	18.27
25	222	17.93
30	227	17.58
35	237	17.26
40	251	16.92
45	265	16.60

This table follows the U. S. standard atmosphere, 1976.

c. Forward and Reverse Reactions. In some cases there are no data on a reaction of interest but there are data on the "reverse" reaction. Occasionally, for

$$A \rightarrow B \ (f)$$
$$B \rightarrow A \ (r)$$

an evaluation will use the data on the "reverse" reaction together with an equilibrium constant to obtain the other rate constant. Obviously this is an approximation but it often is a useful method of estimating non-measured physical properties.

The table contains notations to warn the reader when this procedure has been used, such as "based on reverse reaction," or when both reactions f and r are listed together "$k_f = k_r K_{eq}$" or $k_r = k_f/K_{eq}$. These expressions, which are those used in the analyses, are based on equating the two rates at equilibrium.

$$R_f = R_r$$

$$k_f[A] = k_r[B]$$

$$K_{eq} = [B]/[A] = k_f/k_r.$$

2.4 Convention Concerning Optical Absorption Coefficients

These are reported in the table as "absorption cross sections per molecule, base e". They are defined by the equations.

$$I/I_o = \exp(-\sigma[N]\ell)$$

$$\sigma = (1/([N]\ell))\ln (I_o/I)$$

where I_o and I are the intensities of incident and transmitted light, σ is the absorption cross section, $cm^2 molecule^{-1}$, [N] is the concentration of absorbers, molecules cm^{-3}, and ℓ is the path length, cm. Other definitions and units are frequently used. The terms "absorption coefficient" and "extinction coefficient" are common. It is always necessary to know what concentration units, path length units and type of logarithm (base e or base 10) are used in the definition. To convert "cross-sections" to absorption coefficients in $(atm \text{ at } 273 \text{ K})^{-1} \text{ cm}^{-1}$, base e, multiply by 2.69×10^{19}.

A table of conversion factors is given in the appendix.

3. Arrangement of the Table

Data on a reaction appear only once in the table. The normal location for a reaction is determined by its reactants. Each species has been assigned a sequence number (1 to 65) as shown in the index that follows. These sequence numbers are the same as those used in NBS Technical Note 866. New species have been inserted in appropriate positions and assigned sequence numbers such as 34a, 34b, etc. A reaction is filed under the lower numbered species. That is, the reaction of ozone (7) with an oxygen atom (1) is filed under reactions of oxygen atoms. The numbers for the reactants appear at the left margin of the table, preceding the statement of the reaction, e.g. 1,7 $O + O_3 \rightarrow O_2 + O_2$. These number pairs run in ascending order through the table.

If a reaction is not filed in the location described above, a cross reference is given there. The most common exception is the listing together of data on the forward and reverse reactions of a pair, i.e. $A \rightarrow B$, $B \rightarrow A$.

In the index that follows, bimolecular reactions are listed under <u>both</u> reactants. Frequently the listing of reaction partners for a particular species is divided into two parts by three dashes, separating species earlier in the list than the species indexed from those later in the list. Reactions of the particular species with those species listed before the three dashes should be sought under those reaction partners. There is no indexing of products of reactions. A few species are listed in the index for which there are no reactions in the table, in anticipation of expansion of the data set.

REACTION INDEX

1. O Rxn with: O, $O(^1S)$, O_2, O_3, N, NO, NO_2, NO_3, N_2, N_2O, N_2O_5, NH_2, NH_3, H, HO, HO_2, H_2, H_2O, H_2O_2, HNO_2, HNO_3, SO, SO_2, SO_3, HS, H_2S, CS, CS_2, OCS, ClO, BrO, OClO, HCl, HBr, NO_3Cl, Cl_2, Cl_2O, CO, CO_2, CN, CHO, CH_2O, CH_3, CH_3NO_2, CH_3ONO, CH_4, C_2H_4, C_2H_6, C_3H_6, alkane, C_6H_6, $C_6H_5CH_3$, CH_3Cl

2. $O(^1D)$ Rxn with: O_2, O_3, NO, NO_2, N_2, N_2O, NH_3, H_2, H_2O, H_2O_2, HCl, CO_2, CH_4, C_2H_6, CF_2Cl_2, $CFCl_3$

3. $O(^1S)$ Rxn with: O, O_2, O_3, NO, NO_2, N_2, N_2O, NH_3, H_2O, CO_2, CH_4

4. O_2 Rxn with: O, $O(^1D)$, $O(^1S)$ - - -
hν, N, NO, NO_2, NO_3, N_2, H, H_2, H_2O, H_2O_2, HNO, SO, HS, Cl, CN, CHO, CH_3, CH_3O

5. $O_2(^1\Delta)$ Rxn with: O_2, O_3, N, NO, N_2, H, SO, SO_2, H_2S, CO, CF_2Cl_2, CCl_4, CH_3Cl, CH_2Cl_2, $CHCl_3$

6. $O_2(^1\Sigma)$ Rxn with: O_2, N_2, H_2O

7. O_3 Rxn with: O, $O(^1D)$, $O(^1S)$, $O_2(^1\Delta)$ - - -
hν, M, N, NO, NO_2, H, HO, HO_2, SO, SO_2, H_2S, Cl, Br, ClO, BrO, CO, CH_2O, CH_3, CH_3O_2, CH_3ONO, CH_4, C_2H_4, C_3H_6, allene, butenes, butadiene, $C_2Cl_2H_2$

8. N Rxn with: O, O_2, $O_2(^1\Delta)$, O_3 - - -
N, NO, NO_2, HO, SO, SO_3, OClO

9. NO Rxn with: O, $O(^1D)$, $O(^1S)$, O_2, $O_2(^1\Delta)$, O_3, N - - -
$h\nu$, M, NO, NO_2 + H_2O, NO_3, NH, NH_2, H, HO,
HO_2, H_2, H_2O, H_2O_2, Cl, ClO, BrO, OClO,
CH_3, CH_3O, CH_3O_2

10. NO_2 Rxn with: O, $O(^1D)$, $O(^1S)$, O_2, O_3, N, NO + H_2O - - -
$h\nu$, M, NO_2, NO_3, NH_2, NH_3, H, HO, HO_2,
SO_2, Cl, ClO, CH_3, CH_3O, CH_3O_2

11. NO_3 Rxn with: O, O_2, NO, NO_2 - - -
$h\nu$, M, NO_3, H_2O, SO_2

12. N_2 Rxn with: O, $O(^1D)$, $O(^1S)$, O_2, $O_2(^1\Delta)$, $O_2(^1\Sigma)$ - - -
M, HO

13. N_2O Rxn with: O, $O(^1D)$, $O(^1S)$ - - -
$h\nu$, M, H, HO, ClO, CO

14. N_2O_5 Rxn with: O - - - $h\nu$, M, H_2O, SO_2

15. NH Rxn with: NO - - -

16. NH_2 Rxn with: O, NO - - - H, HO, H_2, H_2O

17. NH_3 Rxn with: O, $O(^1D)$, $O(^1S)$, NO_2 - - -
M, H, HO, ClO

17a. N_2H_4 Rxn with: H

18. H Rxn with: O, O_2, $O_2(^1\Delta)$, O_3, NO, NO_2, N_2O, NH_2, NH_3, N_2H_4 - - -
H, HO, HO_2, H_2O, H_2O_2, HNO, HNO_2, HNO_3, SO_2, HS, H_2S, COS, OClO, HCl, NOCl, Cl_2, CO, CO_2, CH_2O, CH_3OOH, CH_3ONO, CH_3Cl

19. HO Rxn with: O, O_3, N, NO, NO_2, N_2, N_2O, NH_2, NH_3, H - - -
M, HO, HO_2, H_2, D_2, H_2O, H_2O_2, HNO, HNO_2, HNO_3, SO_2, H_2S, Cl, HCl, DCl, HBr, NO_3Cl, CO, CH_2O, CH_3OH, CH_3NO_2, CH_3ONO, CH_4, C_2H_2, C_2H_4, C_2H_6, C_3H_6, C_4H_{10}, alkane, C_6H_6, $C_6H_5CH_3$, CF_2Cl_2, $CFCl_3$, CCl_4, CH_3Cl, CH_2Cl_2, $CHCl_3$, $CH_iCl_jF_k$

20. HO_2 Rxn with: O, O_3, NO, NO_2, H, HO - - -
M, HO_2, H_2, H_2O, SO_2, Cl, Br, ClO, CO, CH_2O, CH_3O_2, C_2H_4, C_2H_6, C_3H_8, C_4H_{10}

21. H_2 Rxn with: O, $O(^1D)$, O_2, NO, NH_2, HO, HO_2 - - -
M, Cl, ClO

22. H_2O Rxn with: O, $O(^1D)$, $O(^1S)$, O_2, $O_2(^1\Sigma)$, NO, NO_3, N_2O_5, NH_2, H, HO, HO_2 - - - SO_3

23. H_2O_2 Rxn with: O, $O(^1D)$, O_2, NO, H, HO - - -
$h\nu$, M, Cl, Br

24. HNO Rxn with: O_2, H, HO - - - M, HNO

25. HNO_2 Rxn with: O, H, HO - - - $h\nu$

26. HNO_3 Rxn with: O, H, HO - - - $h\nu$, M, Cl

26a. S Rxn with: CS_2, COS

27. SO Rxn with: O, O_2, $O_2(^1\Delta)$, O_3, N - - - SO, SO_3

28. SO_2 Rxn with: O, $O_2(^1\Delta)$, O_3, NO_2, NO_3, N_2O_5, H, HO, HO_2 - - - CH_3

29. SO_3 Rxn with: O, N, H_2O, SO - - -

30. S_2O Rxn with:

31. HS Rxn with: O, O_2, H - - - HS

32. H_2S Rxn with: O, $O_2(^1\Delta)$, O_3, H, HO - - -

33. HSO_3 Rxn with:

34. H_2SO_4 Rxn with:

34a. CS Rxn with: O - - -

34b. CS_2 Rxn with: O, S - - -

34c. COS Rxn with: O, H, S - - -

35. Cl Rxn with: O_2, O_3, NO, NO_2, HO, HO_2, H_2, H_2O_2, HNO_3 - - - Cl, OClO, ClOO, NOCl, NO_2Cl, NO_3Cl, Cl_2O, CH_4, C_2H_6

Br Rxn with: O_3, HO_2, H_2O_2 - - -

36. ClO Rxn with: O, O_3, NO, NO_2, N_2O, NH_3, HO_2, H_2 - - - $h\nu$, ClO, BrO, CO, CH_4, C_2H_2, C_2H_4

BrO Rxn with: O, O_3, NO, ClO - - - BrO

37. ClOO Rxn with: Cl - - - $h\nu$, M

OClO Rxn with: O, N, NO, H, Cl - - - $h\nu$

38. ClO_3 Rxn with:

39. HCl Rxn with: O, $O(^1D)$, H, HO - - - $h\nu$

HBr Rxn with: O, HO - - -

40. HOCl Rxn with: $h\nu$

41. HOClO Rxn with:

42. NOCl Rxn with: H, Cl - - - $h\nu$

43. NO_2Cl Rxn with: Cl - - - $h\nu$

43a. NO_3Cl Rxn with: O, HO, Cl - - - $h\nu$

44. Cl_2 Rxn with: O, H - - - $h\nu$

44a. Cl_2O Rxn with: O, Cl - - -

45. CO Rxn with: O, $O_2(^1\Delta)$, O_3, N_2O, H, HO, HO_2, ClO - - - CH_3O

46. CO_2 Rxn with: O, $O(^1D)$, $O(^1S)$, H - - - M

46a. CN Rxn with: O, O_2 - - -

47. CHO Rxn with: O, O_2 - - -

48. CH_2O Rxn with: O, O_3, H, HO, HO_2 - - - $h\nu$

49. CH_3 Rxn with: O, O_2, O_3, NO, NO_2, SO_2 - - -

50. CH_3O Rxn with: O_2, NO, NO_2, CO

51. CH_3O_2 Rxn with: O_3, NO, NO_2, HO_2 - - - CH_3O_2

52. CH_3OH Rxn with: HO - - -

53. CH_3OOH Rxn with: H - - -

54. CH_3NO_2 Rxn with: O, HO - - -

CH_3ONO Rxn with: O, O_3, H, HO - - - $h\nu$

55. CH_3NO_3 Rxn with:

56. CH_4 Rxn with: O, $O(^1D)$, $O(^1S)$, O_3, HO, Cl, ClO - - -

56a. C_2H_2 Rxn with: HO, ClO - - -

57. C_2H_4 Rxn with: O, O_3, HO, HO_2, ClO - - -

58. C_2H_6 Rxn with: O, $O(^1D)$, HO, HO_2, Cl - - -

*59. C_3H_6 Rxn with: O, O_3, HO - - -

†60. C_3H_8 Rxn with: O, HO, HO_2 - - -

∇60a. C_6H_6 Rxn with: O, HO - - -

61. CF_2Cl_2 Rxn with: $O(^1D)$, $O_2(^1\Delta)$, HO - - - hν

62. $CFCl_3$ Rxn with: $O(^1D)$, HO - - - hν

63. CCl_4 Rxn with: HO - - - hν

64. CH_iCl_j Rxn with: O, $O_2(^1\Delta)$, O_3, H, HO - - -

✓65. $CH_iCl_jF_k$ Rxn with: HO - - -

* and higher alkenes
† and higher alkanes
∇ and other aromatics
✓ and other halocarbons

No.	Reaction/Reference * = Preferred Value + = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant k/cm^{3}molecule^{-1}s^{-1}	Notes and Reliability of log k
1,1M	$O + O + M \rightarrow O_2 + M$			
	*Campbell, Gray (1973)	298	4.8×10^{-33} M = N_2	±0.03
		196	11.1×10^{-33}	±0.02
	*Johnston (1968) review	1000-8000	$3.80 \times 10^{-30}\ T^{-1} \exp(-170/T)$ M = O_2	±0.3
	Taylor (1975) review	2000-10000	$1.7 \times 10^{-32}\ T^{-1/2}$ M = N_2	
			$2.2 \times 10^{-28}\ T^{-3/2}$ M = O_2	
			$6.2 \times 10^{-28}\ T^{-3/2}$ M = O	
			$8.3 \times 10^{-33}\ T^{-1/2}$ M = N, NO	
	Baulch, et al (1976) review	190-4000	$5.2 \times 10^{-35} \exp(900/T)$ M = Ar	±0.1 at 190K
1,3	$O + O(^1S) \rightarrow$		see $O(^1S) + O \rightarrow$	
1,4M	$O(^3P) + O_2 + M \rightarrow O_3 + M$ (f)			
7,M	$O_3 + M \rightarrow O + O_2 + M$ (r)			
	*This Survey	200-346	$k_f = 6.6 \times 10^{-35} \exp(510/T)$ M = Ar Rel. M eff.: Ar(1.0), N_2(1.6), O_2(1.7), H_2O(15)	±.07
	Baulch, et al (1976) review	300	$k_f = 5.5 \times 10^{-34}$ M = N_2	
		200-1000	$k_r = 4.1 \times 10^{-10} \exp(-11430/T)$ M = Ar	
	Johnston (1968) eval.	200-1000	$k_f = 4.6 \times 10^{-35} \exp(1050/T)$ M = O_2	±0.1
			$k_r = 1.65 \times 10^{-9} \exp(-11400/T)$cm^{3}molecule^{-1}s^{-1} Rel. M eff.: O_3(1.0), Ar(0.25), O_2(0.44), N_2(0.30)	±0.1
	Huie, Herron, Davis (1972)	200-346	$k_f = 6.6 \times 10^{-35} \exp(510/T)$ M = Ar Rel. M efficiencies: Ar(1.0), He(0.9), N_2(1.7)	
	Mulcahy, Williams (1968)	213-386	$k_f = 4.7 \times 10^{-35} \exp(840/T)$ M = Ar Rel. M eff.: Ar(1.0), He(0.8), CO_2(3.4), O_2(1.1)	
	Meaburn, et al (1968)	300	$k_f = 1.0 \times 10^{-33}$ M = CO_2 Rel. M eff.: CO_2(1.0), CO(0.44), N_2O(0.88)	
	Stuhl, Niki (1971)	300	$k_f = 5.4 \times 10^{-34}$ cm^{6}molecule^{-2}s^{-1} M = N_2 Rel. M efficiencies: N_2(1.0) O_2(1.18), CO(1.24)	
	Donovan, Husain, Kirsch (1970)	300	$k_f = 5.0 \times 10^{-34}$ cm^{6}molecule^{-2}s^{-1} M = Ar Rel. M efficiencies: Ar(1.0), Kr(0.98), He(0.92)	
	Hippler, Troe (1971)	300	$k_f = 8 \times 10^{-34}$ M = N_2	
	Slanger, Black (1970)	300	$k_f = 4.4 \times 10^{-34}$ M = Ar, Rel. eff. Ar(1.0), N_2(1.6)	
	Francis (1969)	300	$k_f = 1.24 \times 10^{-34}$ M = O_2	
	Sauer (1967)	300	$k_f = 2.28 \times 10^{-34}$ M = Ar	
	Ball and Larkin (1973)	295	$k_f = 5.4 \pm 1.2 \times 10^{-34}$ M = N_2 Rel. efficiencies: N_2(1.0), O_2(1.09), Ar(0.78)	
	Hippler, Schippert, Troe (1975)	300	$k_f \sim 8 \times 10^{-34}$ cm^{6}molecule^{-2}s^{-1} M = N_2	(a)
			$k_{f(-)} = 2.8 \times 10^{-12}$ cm^{3}molecule^{-1}s^{-1}	(a,b)

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
			(a) Reevaluation of work in Hippler, Troe (1971) (b) 2d order high pressure limit	
	Hogan, Burch (1976)	300	6.3×10^{-34} M = O_2	
1,4M	$O + O_2 + M \rightarrow O_3^* + M$			
	Bevan, Johnson (1973)	300	$5.4 \times 10^{-34} cm^6 molecule^{-2} s^{-1}$ M = O_2 Rel. efficiencies: O_2(1.0), Ar(0.50), N_2O(2.4), CO_2(2.5), SF_6(5.7)	(a)
	von Rosenberg, Trainor (1974)	300	$3 \times 10^{-34} cm^6 molecule^{-2} s^{-1}$ (a) Vibrationally excited O_3 followed as fn. of time using absn. 250 < λ <330nm. (b) Vibrationally excited O_3 followed as fn. of time using i.r. emission at 9.6 and 14.3 μm Also see von Rosenberg, Trainor (1975)	(b)
1,7	$O(^3P) + O_3 \rightarrow O_2 + O_2$			
	*Hampson (1973) eval.	220-1000	$1.9 \times 10^{-11} \exp(-2300/T)$	±0.1
	Baulch, et al (1976) review	200-500	$8.6 \times 10^{-12} \exp(-2090/T)$	±0.2
	McCrumb, Kaufman (1972)	269-409	$1.1 \times 10^{-11} \exp(-2155/T)$	
	Lundell, Ketcheson, Schiff (1969)	300	1.5×10^{-14}	
	Husain, Kirsch, Donovan (1972)	300	1.3×10^{-14}	
	Davis, Wong, Lephardt (1973)	220-353	$2.0 \times 10^{-11} \exp(-2280/T)$	
1,8M	$O + N + M \rightarrow NO + M$			
	*Baulch, et al (1973) review	200-400	$1.8 \times 10^{-31} (T)^{-0.5} cm^6 molecule^{-2} s^{-1}$, M = N_2	±0.?
	Taylor (1975)	2000-10000	$2.8 \times 10^{-28} T^{-3/2}$ M = N_2, O_2, N, O $5.5 \times 10^{-27} T^{-3/2}$ M = NO	
	Campbell, Gray (1973)	298	9.2×10^{-33}	
		196	12.1×10^{-33}	
1,9	$O + NO \rightarrow N + O_2$ (f)			
4,8	$O_2 + N \rightarrow NO + O$ (r)			
	*Baulch, et al (1973) review	1000-3000	$k_f = 2.5 \times 10^{-15} T \exp(-19500/T)$	±0.12 at 1000K (a)
	†*Becker, Groth, Kley (1969)	280-333	$k_r = 5.5 \times 10^{-12} \exp(-3200/T)$	±0.2 at 230K
	Baulch, et al (1973) review	300-3000	$k_r = 1.1 \times 10^{-14} T \exp(-3150/T)$	±0.12 at 300<T<1500K
			(a) $k_f = k_r K_{eq}$. Error in log k increases to ±0.3 at 3000K	
	Taylor (1975)	2000-10000	$k_r = 2.2 \times 10^{-14} (T) \exp(-3560/T)$	
1,9	$O + NO \rightarrow NO_2 + h\nu$			
	Becker, et al (1973)	300	4.2×10^{-18}	
1,9M 10,M	$O + NO + M \rightarrow NO_2 + M$ (f) $NO_2 + M \rightarrow NO + O + M$ (r)			
	†*Whytock, Michael, Payne (1976)	220-500	$k_f = 1.55 \times 10^{-32} \exp(584/T) cm^6 molecule^{-2} s^{-1}$, M = N_2	±0.?
	Baulch, et al (1973) review	200-500	$k_f = 3.0 \times 10^{-33} \exp(940/T) cm^6 molecule^{-2} s^{-1}$, M = O_2 Rel. M efficiencies: O_2(1.0), Ar(1.0), N_2(1.4)	±0.08
		1400-2400	$k_r = 1.8 \times 10^{-8} \exp(-33000/T) cm^3 molecule^{-1} s^{-1}$	±0.1

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
			M = Ar	
	Slanger, Wood, Black (1973)	296	$k_f = 6.0 \times 10^{-32}$ M = Ar	
		241	$k_f = 13.0 \times 10^{-32}$ M = Ar	
	Hippler, Schippert, Troe (1975)	300	$k_f = 7.4 \times 10^{-32}$ $cm^6 molecule^{-2} s^{-1}$ M = N_2	
			$k_{f(\infty)} = 3.0 \times 10^{-11}$ $cm^3 molecule^{-1} s^{-1}$	(a)
			(a) 2d order high pressure limit	
	Atkinson, Pitts (1974)	300-392	$k_f = 2.6 \times 10^{-32} \exp(450 \pm 100/T)$ M = N_2	
	Singleton, et al (1975)	298-473	$k_f = 1.7 \times 10^{-32} \exp(620/T)$, M = N_2	
	Campbell, Handy (1976)	285-425	$k_f = 5.0 \times 10^{-33} \exp(900/T)$, M = N_2	
	Michael, Payne, Whytock (1976)	217-500	$k_f = 1.08 \times 10^{-32} \exp(520/T)$, M = He	
			$k_f = 9.33 \times 10^{-33} \exp(515/T)$, M = Ne	
			$k_f = 9.01 \times 10^{-33} \exp(590/T)$, M = Ar	
			$k_f = 9.52 \times 10^{-33} \exp(570/T)$, M = Kr	
1,9M	O + NO + M → NO_2 + M + hν			
	Becker, et al (1973)	300	7×10^{-32} $cm^6 molecule^{-2} s^{-1}$	
1,10	$O(^3P)$ + NO_2 → NO + O_2 (f)			
4,9	O_2 + NO → NO_2 + O (r)			
	†*Davis, Herron, Huie (1973)	230-339	$k_f = 9.1 \times 10^{-12}$	±0.06
	Baulch, et al (1973)	300-550	$k_f = 1.7 \times 10^{-11} \exp(-300/T)$	
			$k_r = k_f/K_{eq} = 2.8 \times 10^{-12} \exp(-23400/T)$	±0.1
	Clyne, Cruse (1971)	300	$k_f = 8.3 \times 10^{-12}$	
	Harker, Johnston (1973)	300	$k_f = 9.2 \times 10^{-12}$	(a)
	Clyne, Cruse (1972)	298	$k_f = 6.1 \times 10^{-12}$	
	Slanger, et al (1973)	300	$k_f = 9.3 \times 10^{-12}$	(b)
		240	$k_f = 10.5 \times 10^{-12}$	
	Hampson, et al (1973a) review	220-500	$k_f = 9.1 \times 10^{-12}$	±0.08
	Stuhl, Niki (1970)	300	$k_f = 4.4 \times 10^{-12}$	(b)
	Bemand, Clyne, Watson (1973)	230-1055	$k_f = 1.75 \times 10^{-10} \times (T)^{-0.52}$	(c)
		298	$k_f = 9.5 \pm 1.1 \times 10^{-12}$	
			(a) k/k(O + NO + M) measured, where k(ref) = 6.9×10^{-32}	
			(b) Similar techniques were used by Slanger and by Stuhl and Niki: Flash photolysis - chemiluminescence.	
			(c) Based on this work ($298 < T/K < 1055$) and other recent work.	
1,10M	O + NO_2 + M → NO_3 + M (f)			
11,M	NO_3 + M → NO_2 + O + M (r)			
	*Hampson, et al (1973a) review	298	$k_f = 1.0 \times 10^{-31}$ cm^6 $molecule^{-2} s^{-1}$ M = N_2	±0.2
	Baulch, et al (1973) review	295	$k_f = 6.3 \times 10^{-32}$ M = N_2	±0.4

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
			$k_r \sim 8 \times 10^{-42}$ $cm^3 molecule^{-1} s^{-1}$, M = N_2	(a)
	Hippler, Schippert, Troe (1975)	300	$k_f = 8.0 \times 10^{-32}$ $cm^6 molecule^{-2} s^{-1}$ M = N_2	
			$k_{f(\infty)} = 2.0 \times 10^{-11}$ $cm^3 molecule^{-1} s^{-1}$	(b)
			(a) No reliable data. Value based on k_f	
			(b) 2d order high pressure limit	
1,11	$O + NO_3 \rightarrow O_2 + NO_2$			
	Graham, Johnston (1978)	300	$(1.0 \pm 0.4) \times 10^{-11}$	
1,12	$O + N_2 \rightarrow N + NO$		see reverse reaction	
1,12M	$O + N_2 + M \rightarrow N_2O + M$ (f)			
13,M	$N_2O + M \rightarrow N_2 + O + M$ (r)			
	Baulch, et al (1973) review	1300-2500	$k_f = 3.9 \times 10^{-35} \exp(-10400/T)$ $cm^6 molecule^{-2} s^{-1}$	
			M = Ar	±0.2 (a)
			$k_r = 8.3 \times 10^{-10} \exp(-29000/T)$ $cm^3 molecule^{-1} s^{-1}$	
			M = Ar	±0.2
		900-2100	$k_f = 5.5 \times 10^{-15} \exp(-11330/T)$ $cm^3 molecule^{-1} s^{-1}$	±0.2 (a,b)
			$k_r = 1.3 \times 10^{+11} \exp(-30000/T) s^{-1}$	±0.2 (c)
			(a) $k_f = k_r K_{eq}$	
			(b) 2d order high pressure limit	
			(c) 1st order high pressure limit	
	Schofield (1973) review	300-568	$k_f \leq 5 \times 10^{-38}$ $cm^6 molecule^{-2} s^{-1}$	upper limit only
		800-2100	$k_{r\infty} = 1.4 \times 10^{11} \exp(-30,000/T) s^{-1}$	1st order limit
1,13	$O + N_2O \rightarrow N_2 + O_2$ (1)			
1,13	$O + N_2O \rightarrow NO + NO$ (2)			
9,9	$NO + NO \rightarrow N_2O + O$ (2r)			
	Baulch, et al (1973) review	1200-2000	$k_1 = 1.7 \times 10^{-10} \exp(-14.1 \times 10^3/T)$	±0.4 (a)
			$k_2 = 1.7 \times 10^{-10} \exp(-14.1 \times 10^3/T)$	±0.3
		1200-2000	$k_{2r} = 2.2 \times 10^{-12} \exp(-32100/T)$	±0.3 (b)
			(a) Based on $k_1/k_2 = 1$	
			(b) $d[NO]/dt = -2k_{2r}[NO]^2$	
	Taylor (1975) review	2000-10000	$k_{2r} = 0.4T^{-5/2} \exp(-43000/T)$	
1,14	$O + N_2O_5 \rightarrow$ products			
	Graham, Johnston (1978)	300	$< 2 \times 10^{-14}$	
	Davis (1974)	300	$< 2 \times 10^{-13}$	preliminary
1,16	$O + NH_2 \rightarrow HNO + H$ (a)			
	$\rightarrow HO + NH$ (b)			
	Gehring, et al (1973)	300	3.5×10^{-12} $(k_a + k_b)$	
1,17	$O + NH_3 \rightarrow HO + NH_2$ (f)			
16,19	$HO + NH_2 \rightarrow O + NH_3$ (r)			
	*Kurylo, et al (1969)	361-677	$k_f = 6.6 \times 10^{-12} \exp(-3300/T)$	±0.3
	Baulch, et al (1973) review	300-1000	$k_f = 2.5 \times 10^{-12} \exp(-3020/T)$	±0.2
		300-1000	$k_r = k_f/K_{eq} = 1 \times 10^{-13}$	±0.2 (a)

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
	Albers, et al (1969)	300-1000	$k_f = 2 \times 10^{-12} \exp(-3000/T)$	
	Kondratiev (1970) review	350-1000	$k_f = 1.8 \times 10^{-12} \exp(-2500/T)$ Data of Albers, et al provide an upper limit when extrapolated to 220K (a) $HO + NH_2 \rightarrow NH + H_2O$ may be preferred channel.	
1,18M	$O + H + M \rightarrow HO + M$			
	Schofield (1973) review	1000-3000	$\sim 2 \times 10^{-32}$ $cm^6 molecule^{-2} s^{-1}$ M = Ar	±1 estimate
	Baulch, et al (1972) review		No recommendation	
1,19	$O + HO \rightarrow H + O_2$ (f)			
4,18	$O_2 + H \rightarrow O + HO$ (r)			
	†*Wilson (1972) review	300-2000	$k_f = 4.2 \pm 1.7 \times 10^{-11}$	±0.3
	*Baulch, et al (1972) review	700-2500	$k_r = 3.7 \times 10^{-10} \exp(-8450/T)$	±0.1
	Baulch, et al (1972) review	300	$k_f = 3.8 \pm 1.7 \times 10^{-11}$	±0.17
1,19M	$O + HO + M \rightarrow HO_2 + M$ (f)			
20,M	$HO_2 + M \rightarrow O + HO + M$ (r)			
	Baulch, et al (1972) review		no recommendation for forward or reverse rxn	
1,20	$O + HO_2 \rightarrow HO + O_2$			
	†*Burrows, Harris, Thrush (1977)	293	3.5×10^{-11} (a) Based on value for $k(O + HO)$ and $k(HO + H_2O_2)$	±0.3 at 230K (a)
	Lloyd (1974) review	~300	$8 \times 10^{-11} \exp(-500/T)$	estimate
1,21	$O + H_2 \rightarrow HO + H$ (f)			
18,19	$H + HO \rightarrow O + H_2$ (r)			
	Baulch, et al (1972) review	400-2000	$k_f = 3.0 \times 10^{-14}(T)\exp(-4480/T)$	±0.1
			$k_r = k_f/K_{eq} = 1.4 \times 10^{-14}(T)\exp(-3500/T)$	±0.15
	Dubinsky, McKenney (1975)	347-742	$k_f = 8.8 \times 10^{-12} \exp(-4200/T)$	
	Schott, et al (1974)	1400-1900	$k_f/k_{ref} = 3.6 \pm 0.7$ Ref rxn is $O_2 + H \rightarrow O + HO$	
	Campbell, Handy (1975)	363-490	$k_f = 5.1 \times 10^{-11} \exp(-4950/T)$	
1,22	$O + H_2O \rightarrow HO + HO$		see reverse reaction	
1,22	$O + H_2O \rightarrow H + HO_2$			
	Baulch, et al (1972) review		no recommendation	
1,23	$O(^3P) + H_2O_2 = HO_2 + OH$ (a) $= H_2O + O_2$ (b)			
	†*Davis, Wong, Schiff (1974)	283-373	$k(a+b) = 2.75 \times 10^{-12} \exp(-2125/T)$	±0.3 (a)
	Foner, Hudson (1962)	300	$\leq 4 \times 10^{-15}$	
	Albers, et al (1971)	370-800	$k(a + b) = 4.6 \times 10^{-11} \exp(-3220/T)$	
			(a) Although there is no evidence, products are most likely $OH + HO_2$ as the channel to produce $H_2O + O_2$ requires a complex rearrangement.	
1,25	$O + HNO_2 \rightarrow HO + NO_2$			
	This survey		No data. Probably faster than $O + HNO_3$, since it is 94 kJ/mol more exothermic.	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
1,26	$O + HNO_3 \rightarrow HO + NO_3$			
	*Chapman, Wayne (1974)	300	$< 3 \times 10^{-17}$	
	Hampson, et al (1973) review	300	$< 1.5 \times 10^{-14}$	
	Morley, Smith (1972)	300	$< 1.3 \times 10^{-14}$	
	Baulch, et al (1973) review	300	$< 10^{-14}$	approximate upper limit
1,27	$O + SO \rightarrow SO_2 + h\nu$			
	Baulch, et al (1976) review		no recommendation	
1,27M	$O + SO + M \rightarrow SO_2 + M$ (f)			
28,M	$SO_2 + M \rightarrow O + SO + M$ (r)			
	*Baulch, et al (1976) review	298	$k_f = 1.9 \times 10^{-31}$ $cm^6 molecule^{-2} s^{-1}$ M = Ar k_r no recommendation	±0.15
	Schofield (1973) review	300	$k_f = 8.8 \times 10^{-31}$, M = Ar	±0.3
		4500-7500	$k_r = 4.2 \times 10^{-10} \exp(-55000/T)$	±0.3
1,28	$O + SO_2 \rightarrow O_2 + SO$ (f)			
4,27	$O_2 + SO \rightarrow O + SO_2$ (r)			
	*Baulch, et al (1976) review	440-2100	$k_f = 2.1 \times 10^{-10} T^{-0.5} \exp(-9980/T)$	±0.25 (a)
		440-2100	$k_r = 7.5 \times 10^{-13} \exp(-3250/T)$	±0.25
	Breckenridge, Miller (1972)	300	$k_r = < 8 \times 10^{-17}$	
	Schofield (1973) review	400-2500	$k_r = 3.0 \times 10^{-13} \exp(-2800/T)$ (a) $k_f = k_r \times K_{eq}$	±0.3
1,28M	$O + SO_2 + M \rightarrow SO_3 + M$			
	*Davis (1976)	220-353	$3.4 \times 10^{-32} \exp(-1130/T)$ $cm^6 molecule^{-2} s^{-1}$ M = N_2 N_2(1.0), He(.45), Ar(.87), SO_2(56)	
	Schofield (1973) review	250-1000	$1 \times 10^{-33} \exp(\pm 500/T) cm^6 molecule^{-2} s^{-1}$ M = O_2, N_2, Ar, He	±0.3 at 300K ±0.6 at other temp.
	Atkinson, Pitts (1974)	299-392	$9.2 \times 10^{-32} \exp(-1000/T)$, M = N_2O	
	Westenberg, deHaas(1975d)	248-415	$1.07 \times 10^{-31} \exp(-1400/T)$, M = He Rel. eff: He(1.0), N_2(2.4), SO_2(9.5)	
	Baulch, et al (1976) review		no recommendation	
1,29	$O + SO_3 \rightarrow$ products			
	Westenberg, deHaas (1975c)	298-507	$1.4 \times 10^{-31} \exp(785/T)$ $cm^6 molecule^{-2} s^{-1}$ Rel. eff: He(1.0), N_2(1.4) (a) Reaction $O + SO_3 + M \rightarrow$ products found to be 3rd order up to P = 7 Torr; SO_4 not detected	(a)
	Schofield (1973) review	1480-1550	$5 \times 10^{-10} \exp(-6000/T)$	uncertain
	Jacob, Winkler (1972)	300-500	$3 \times 10^{-16} \exp(-500/T)$	
	Baulch, et al (1976) review		no recommendation	
1,31	$O + HS \rightarrow H + SO$			
	Cupitt, Glass (1975)	295	$1.6 \pm 0.5 \times 10^{-10}$	
1,32	$O + H_2S \rightarrow HO + HS$			
	*Whytock, et al (1976)	263-495	$7.24 \times 10^{-12} \exp(-1660/T)$	±0.1

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant k/cm^{3}molecule^{-1}s^{-1}	Notes and Reliability of log k
	Hollinden, Kurylo, Timmons (1970)	205-300	$2.9 \times 10^{-13} \exp(-750/T)$	(a)
	Baulch, et al (1976) review		no recommendation	
	Schofield (1973) review	200-350	$6.3 \times 10^{-13} \exp(-920/T)$ (a) Assumes stoichiometry of 3.5	±0.3
1,34a	O + CS → CO + S			
	*Baulch, et al (1976) review	300	2.2×10^{-11}	±0.2
	Bida, et al (1976)	300	2.24×10^{-11}	
	Slagle, et al (1975)	305	2.06×10^{-11}	
1,34b	O + CS_2 → CS + SO (a) → OCS + S (b)			
	*Baulch, et al (1976) review	200-1000	$k_a = 3.7 \times 10^{-11} \exp(-700/T)$	±0.15, T<360K
	Wei, Timmons (1975)	218-293	$k = 2.8 \times 10^{-11} \exp(-640/T)$	
	Slagle, et al (1974)	302	$k = 4.0 \times 10^{-12}$ $k_b/k = 0.093$	
	Graham, Gutman (1976)	249-500	k_b/k decreases from 0.098 at 249K to 0.081 at 500K	
1,34c	O + OCS → SO + CO			
	Manning, et al (1976)	296	$1.10 \pm 0.1 \times 10^{-14}$, P = 50 Torr $1.49 \pm 0.1 \times 10^{-14}$, P = 2 torr	
	Wei, Timmons (1975)	239-404	$2.0 \times 10^{-11} \exp(-2150/T)$	
	Klemm, Stief (1974)	263-502	$1.65 \times 10^{-11} \exp(-2165/T)$	
	Baulch, et al (1976) review	190-1200	$2.6 \times 10^{-11} \exp(-2250/T)$	±0.2 T < 600K ±0.5 T < 600K
1,36	O + ClO → Cl + O_2			
	†*NASA (1977) eval	200-300	$7.7 \times 10^{-11} \exp(-130/T)$	±0.12
	Clyne, Nip (1976)	220-425	$1.07 \times 10^{-10} \exp(-224/T)$ (a) Selected by Watson (1977) review	(a)
	Zahniser, Kaufman (1977)	218-295	$k/k_{ref} = (1.55 \pm 0.17) \exp(246 \pm 30/T)$ (b) $k_{ref} = k(Cl + O_3)$	(b)
1,36Br	O + BrO → Br + O_2			
	†*NASA (1977) eval	200-300	3×10^{-11}	±0.8 at 230K
1,37	O + OClO → ClO + O_2			
	†*NASA (1977) eval	200-300	$2 \times 10^{-11} \exp(-1100/T)$	±0.6 at 230K (a)
	Bemand, et al (1973)	298	5×10^{-13} (a) Based on room temp value of Bemand, et al	±0.2
1,39	O + HCl → HO + Cl (f)			
19,35	HO + Cl → O + HCl (r)			
	†*Watson (1977) eval	200-300	$k_f = 1.14 \times 10^{-11} \exp(-3370/T)$	±0.3 at 230K
	†*NASA (1977) eval	200-300	$k_r = k_f \times K_{eq} = 1.0 \times 10^{-11} \exp(-2970/T)$	±0.3 at 230K
	Balakhnin, et al (1971)	295-371	$k_f = 1.74 \pm 0.6 \times 10^{-12} \exp(-2260/T)$	
	Brown, Smith (1974)	293-440	$k_f = 2.5 \times 10^{-12} \exp(-2970 \pm 150/T)$	
	Wong, Belles (1972)	356-628	$k_f = 1.9 \pm 0.3 \times 10^{-11} \exp(-3580/T)$	
1,39	O + HCl(v = 1) → HO + Cl (a) → O + HCl(v = 0) (b)			

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant k/cm^{3}molecule^{-1}s^{-1}	Notes and Reliability of log k
	Arnoldi, Wolfrum (1974)	300	$3.6 \pm 1.2 \times 10^{-12}$	(a)
	Brown, Glass, Smith (1975)	196-400	$6.2 \times 10^{-12} \exp(-500/T)$	(a)
			(a) Total rate constant for sum of two reaction paths.	
1,39Br	$O + HBr \rightarrow HO + Br$			
	†*NASA (1977) eval	200-300	$7.6 \times 10^{-12} \exp(-1570/T)$	±0.8 at 230K
	Brown, Smith (1975)	267-430	$4.0 \times 10^{-12} \exp(-1360 \pm 50/T)$	
	Takacs, Glass (1973)	298	$(4.4 \pm 1.0) \times 10^{-14}$	
1,43a	$O + NO_3Cl \rightarrow$ products			
	†*NASA (1977) eval	200-300	$3.0 \times 10^{-12} \exp(-808/T)$	±0.15 (a)
	Molina, et al (1977)	213-295	$3.4 \times 10^{-12} \exp(-840/T)$	
	Kurylo (1977)	225-273	$1.9 \times 10^{-12} \exp(-692/T)$	
	Ravishankara, et al (1977)	245	2×10^{-13}	
			(a) Recommended expression given by Kurylo (1977) based on his work and that of Molina, et al (1977)	
1,44	$O + Cl_2 \rightarrow ClO + Cl$			
	*Clyne, et al (1976)	174-602	$4.2 \times 10^{-12} \exp(-1370/T)$	(a)
			(a) Recommendation based on this study (299-602K) and other recent work. Also recommended by Watson (1977) review.	
1,44a	$O + Cl_2O \rightarrow 2ClO$			
	Watson (1977) review	300	1.4×10^{-11}	±0.1
1,45M	$O + CO + M \rightarrow CO_2 + M$ (f)			
46M	$CO_2 + M \rightarrow O + CO + M$ (r)			
	*Baulch, et al (1976) review	250-500	$k_f = 6.5 \times 10^{-33} \exp(-2180/)$ M = CO	±0.2 at 250K inc. to ±0.5 at 500K
		296	$k_f = 2.3 \times 10^{-36}$ M = N_2 no recommendation for k_r	
1,46 4.45	$O + CO_2 \rightarrow CO + O_2$ (f) $O_2 + CO \rightarrow O + CO_2$ (r)			
	*Baulch, et al (1976) review	1500-3000	$k_f = 2.8 \times 10^{-11} \exp(-26500/T)$	±0.3 (a)
		1500-3000	$k_r = 4.2 \times 10^{-12} \exp(-24000/T)$ (a) $k_f = k_r K_{eq}$	±0.3
1,46a	$O + CN \rightarrow CO + N$			
	Schmatjko, Wolfrum (1976)	295	1.8×10^{-11}	
	Albers, et al (1975)	275-387	2.0×10^{-11}	
1,47	$O + CHO \rightarrow CO_2 + H$ (a) $\rightarrow CO + HO$ (b)			
	*Washida, et al (1974)	297	$2.1 \pm 0.4 \times 10^{-10}$ $(k_a + k_b)$	
1,48	$O + CH_2O \rightarrow CHO + OH$			
	†*NASA (1977) eval	200-300	$2 \times 10^{-11} \exp(-1450/T)$	±0.4 at 230K (a)
	Herron, Huie (1973) review	300	1.5×10^{-13}	±0.15

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
	Mack, Thrush (1973)	300	1.5×10^{-13} (a) "A factor" chosen; E_{act} calc to fit k(300K)	±0.05
1,49	$O + CH_3 \rightarrow CH_2O + H$ (a) $\rightarrow CHO + HO$ (b)			
	Washida, Bayes (1976)	259-341	$k_a = 1.0 \pm 0.2 \times 10^{-10}$	
	Washida, et al (1973)	300	k_b negligible $k_b/k_a < 0.05$	
	Slagle, Pruss, Gutman (1974)	300	$k_a = 1.85 \pm 0.28 \times 10^{-10}$	
	Morris, Niki (1972)	300	$k_a/k(O + \text{tetramethylethylene}) = 1.5$	
	Peeters, Mahnen (1973)	1100-1900	$k_a = 2.2 \times 10^{-10} \exp(-1000/T)$	
	Bowman (1975)	1875-2240	$k_a = 1.7 \times 10^{-10}$	
	Biordi, et al (1975)	1550-1725	$k_a = 1.7 \times 10^{-10}$	
1,54	$O + CH_3NO_2 \rightarrow$ products			
	Campbell, Goodman (1975a)	295	3.3×10^{-15}	
1,54	$O + CH_3ONO \rightarrow$ products			
	Davidson, Thrush (1975)	300-410	$2.3 \times 10^{-11} \exp(-2620/T)$	
1,56	$O + CH_4 \rightarrow$ products			
	*Herron, Huie (1973) review	350-1000	$3.5 \times 10^{-11} \exp(-4550/T)$	±0.11
1,57	$O + C_2H_4 \rightarrow CH_3 + HCO$ (a) $\rightarrow CH_2CO + H_2$ (b)			
	*Herron, Huie (1973) evaluation	200-500	$5.5 \times 10^{-12} \exp(-565/T)$ $(k_a + k_b)$	±0.08
	Pruss, Slagle, Gutman (1974)	300	$k_b = 3.81 \pm 0.95 \times 10^{-14}$ $k_b/(k_a + k_b) = 0.05$	(a)
	Atkinson, Pitts (1974)	300-392	$5.6 \times 10^{-12} \exp(-640 \pm 100/T)$ $(k_a + k_b)$	
	Singleton, Cvetanovic (1976)	298-486	$1.16 \times 10^{-11} \exp(-845/T)$ a) Calculated using above recommended value for $(k_a + k_b)$	
1,58	$O + C_2H_6 \rightarrow$ products			
	*Herron, Huie (1973) evaluation	300-650	$4.1 \times 10^{-11} \exp(-3200/T)$	±0.11
1,59	$O + C_3H_6 \rightarrow$ products			
	*Herron, Huie (1973) evaluation	200-500	$4.1 \times 10^{-12} \exp(-38/T)$	±0.08
	Atkinson, Pitts (1974)	300-392	$3.45 \times 10^{-12} \exp(O \pm 150/T)$	
	Singleton, Cvetanovic (1976)	298-483	$1.26 \times 10^{-11} \exp(-363/T)$	
1,60	$O +$ alkane $\rightarrow HO +$ alkyl radical			
	Herron, Huie (1969)	250-600	$k = [0.8 \exp(-2900/T) N_p + 2.2 \exp(-2250/T) N_s + 2.6 \exp(-1650/T) N_t] \times 10^{-11}$ Where N_p, N_s, and N_t are the number of primary, secondary, and tertiary hydrogen atoms, respectively. Do not use formula for CH_4.	
1,60a	$O + C_6H_6 \rightarrow$ products			
	Colussi, et al (1975)	298-462	$1.81 \times 10^{-11} \exp(-2115/T)$	
	Atkinson, Pitts (1975a)	300-392	$1.84 \times 10^{-11} \exp(-2000/T)$	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
	$O + C_6H_5CH_3 \rightarrow$ products			
	Colussi, et al (1975)	298-462	$3.82 \times 10^{-11} \exp(-1940/T)$	
	Atkinson, Pitts (1975a)	300-392	$1.36 \times 10^{-11} \exp(-1560/T)$	
1,64	$O + CH_3Cl \rightarrow HO + CH_2Cl$			
	Westenberg, deHaas (1975a)	500-1000	$5.8 \times 10^{-11} \exp(-4550/T)$	(a)
	Barassin, Combourieu (1974)	298-443	$2.2 \times 10^{-11} \exp(-3450/T)$	
			(a) Also measured $k(O + CH_3Br)/k(O + CH_3Cl)$ to be unity over same temp. range	
2,4	$O(^1D_2) + O_2 \rightarrow O_2(^1\Sigma_g^+) + O(^3P)$			
	†*Streit, et al (1976)	104-354	$2.9 \times 10^{-11} \exp(67/T)$	0.1
	Fletcher, Husain (1976b)	300	5.3×10^{-11}	
2,7	$O(^1D_2) + O_3 \rightarrow O_2 + O_2$ (a) $\rightarrow O_2 + 2O$ (b)			
	†*Streit, et al (1976)	103-393	2.4×10^{-10} $(k_a + k_b)$	±0.1
	Heidner, et al (1973)	300	2.7×10^{-10} $(k_a + k_b)$	
	†*Cvetanovic (1975) review	300	$k_a/k_b \sim 1$	
2,9	$O(^1D_2) + NO \rightarrow NO + O(^3P)$			
	This survey	300	3.5×10^{-11}	±0.3 (a)
	Heidner, Husain (1973)	300	8.5×10^{-11}	
			(a) 0.41 x k of Heidner and Husain; scaled to match other selected $O(^1D)$ rates	
2,10	$O(^1D_2) + NO_2 \rightarrow NO + O_2$			
	This survey	300	1.0×10^{-10}	±0.2 (a)
	Heidner, Husain (1973)	300	2.3×10^{-10}	
			(a) 0.41 x k of Heidner and Husain; scaled to match other selected $O(^1D)$ rates	
2,12	$O(^1D_2) + N_2 \rightarrow N_2 + O(^3P)$			
	†*Streit, et al (1976)	104-354	$2.0 \times 10^{-11} \exp(107/T)$	±0.1
	Heidner, et al (1973)	300	6.9×10^{-11}	
2,12M	$O(^1D_2) + N_2 + M \rightarrow N_2O + M$			
	†*NASA (1977) eval	300	3.5×10^{-37} $cm^6 molecule^{-2} s^{-1}$	(a)
			(a) Derived from data in Kajimoto and Cvetanovic (1976a) and value of $k(O^1D) + N_2)$ this survey	
2,13	$O(^1D_2) + N_2O \rightarrow N_2 + O_2$ (a) $\rightarrow 2NO$ (b)			
	†*Davidson, et al (1977)	204-359	1.1×10^{-10} $(k_a + k_b)$	0.1
	Heidner, Husain (1973)	300	2.2×10^{-10} $(k_a + k_b)$	
	†*Cvetanovic (1975) review	300	$k_a/k_b = 1$	
2,17	$O(^1D_2) + NH_3 \rightarrow NH_2 + HO$			
	*Davidson, et al (1977)	204-354	2.5×10^{-10}	±0.1
	Fletcher, Husain (1976a)	300	6.3×10^{-10}	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
2,21	$O(^1D_2) + H_2 \rightarrow HO + H$			
	†*Davidson, et al (1977)	204-352	9.9×10^{-11}	
	Heidner, Husain (1973)	300	2.7×10^{-10}	
2,22	$O(^1D_2) + H_2O \rightarrow 2HO$			
	†*Streit, et al (1976)	253-353	2.3×10^{-10}	±0.1
	Heidner, et al (1973)	300	3.0×10^{-10}	
2,23	$O(^1D_2) + H_2O_2 \rightarrow HO + HO_2$			
	Fletcher, Husain (1976a)	300	5.2×10^{-10}	
2,39	$O(^1D_2) + HCl \rightarrow$ products			
	†*Davidson, et al (1977)	199-379	1.4×10^{-10}	±0.1
2,45	$O(^1D_2) + CO \rightarrow CO + O(^3P)$			
	*This survey	300	3×10^{-11}	±0.3 (a)
	Heidner, et al (1973)	300	7.3×10^{-11}	
			(a) 0.41 x k of Heidner, et al; scaled to match other selected $O(^1D)$ rates	
2,46	$O(^1D_2) + CO_2 \rightarrow CO_2 + O(^3P)$			
	*Streit, et al (1976)	139-200	1.2×10^{-10}	±0.1
		200-354	6.8×10^{-11} exp(117/T)	±0.1
	Fletcher, Husain (1976b)	300	1.7×10^{-10}	
2,55	$O(^1D_2) + CH_4 \rightarrow CH_3 + HO$ (a) $\rightarrow CH_2O + H_2$ (b)			
	†*Davidson, et al (1977)	198-357	1.4×10^{-10} ($k_a + k_b$)	
	Heidner, Husain (1973)	300	3.1×10^{-10} ($k_a + k_b$)	
	†*Cvetanovic (1975) review	300	$k_a/k_b = 10$	
2,58	$O(^1D_2) + C_2H_6 \rightarrow$ products			
	*This survey	300	3×10^{-10}	±0.2 (a)
	Fletcher, Husain (1976a)	300	7.3×10^{-10}	
			(a) 0.41 x k of Fletcher and Husain; scaled to match other selected $O(^1D)$ rates	
2,61	$O(^1D_2) + CF_2Cl_2 \rightarrow$ products			
	†*NASA (1977) eval	300	2×10^{-10}	±0.2 (a)
	Fletcher, Husain (1976b)	300	4.8×10^{-10}	
			(a) 0.41 x k of Fletcher and Husain; scaled to match other selected $O(^1D)$ rates	
2,62	$O(^1D_2) + CFCl_3 \rightarrow$ products			
	†*NASA (1977) eval	300	2.3×10^{-10}	±0.2 (a)
	Fletcher, Husain (1976b)	300	5.5×10^{-10}	
			(a) 0.41 x k of Fletcher and Husain; scaled to match other selected $O(^1D)$ rates	
3,1	$O(^1S) + O(^3P) \rightarrow$?			
	Slanger, Black (1976a)	200-365	5×10^{-11} exp(-305/T)	
3,4	$O(^1S) + O_2 \rightarrow$?	200-377	4.3×10^{-12} exp(-850/T)	±0.15 a

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
3,7	$O(^1S) + O_3 \rightarrow ?$	300	5.8×10^{-10}	±0.07 a
3,9	$O(^1S) + NO \rightarrow ?$	200-291	$3.2 \times 10^{-11}(T)^{0.5}$	±0.05 a
3,10	$O(^1S) + NO_2 \rightarrow ?$	300	5×10^{-10}	±0.2 a
3,12	$O(^1S) + N_2 \rightarrow ?$	200-380	$< 5 \times 10^{-17}$	a
3,13	$O(^1S) + N_2O \rightarrow ?$			
	Slanger, Black (1976b)	200-368	$3.8 \times 10^{-11} \exp(-420/T)$	
3,17	$O(^1S) + NH_3 \rightarrow ?$	300	5×10^{-10}	±0.2 a
3,22	$O(^1S) + H_2O \rightarrow ?$			
	Bingham, et al (1976)	300	1.3×10^{-10}	
3,46	$O(^1S) + CO_2 \rightarrow ?$	200-450	$3.1 \times 10^{-11} \exp(-1320/T)$	±0.15 a
3,56	$O(^1S) + CH_4 \rightarrow ?$	300	2×10^{-14}	±0.4 a
			a) Rate constants evaluated for this survey by T. G. Slanger and K. H. Welge (1973).	
4,hν	$O_2 + h\nu \rightarrow O(^3P) + O(^3P)$			
	Hampson, et al (1973a) review		$\phi = 1$ $175 < \lambda < 200$ nm	
4,hν	$O_2 + h\nu \rightarrow O(^3P) + O(^1D)$			
	Hampson, et al (1973a) review		$\phi = 1$ $133 < \lambda < 175$ nm	
4,hν	$O_2 + h\nu \rightarrow$ 2 oxygen atoms			
	Hampson, et al (1973a) review		$\phi = 1$ $106 < \lambda < 200$ nm	
4,hν	$O_2 + h\nu$			
	Hampson, et al (1973a) review		Recommended values of absorption cross section $135 < \lambda < 243$ nm	
4,8	$O_2 + N \rightarrow NO + O$		see reverse reaction	
4,9,9	$O_2 + NO + NO \rightarrow NO_2 + NO_2$		$-d[NO]/dt = d[NO_2]/dt = 2k_1[NO]^2[O_2]$	
	*Baulch, et al (1973) review	273-660	$3.3 \times 10^{-39} \exp(530/T)$ $cm^6 molecule^{-2} s^{-1}$	±0.2
	Stedman, Niki (1973)	300	2.0×10^{-38}	±0.1
4,9,10	$O_2 + NO + NO_2 \rightarrow NO_2 + NO_3$		see reverse reaction	
4,9	$O_2 + NO \rightarrow NO_2 + O$		see reverse reaction	
4,9M	$O_2 + NO + M \rightarrow NO_3 + M$			
	Baulch, et al (1973) review		No recommendation	
4,10	$O_2 + NO_2 \rightarrow NO + O_3$		see reverse reaction	
4,11	$O_2 + NO_3 \rightarrow NO_2 + O_3$		see reverse reaction	
4,12	$O_2 + N_2 \rightarrow N_2O + O$			
	*Baulch, et al (1973) review	1200-2000	$1.0 \times 10^{-10} \exp(-55.2 \times 10^3/T)$	±0.4 (a)
			(a) $k_f = k_r K_{eq}$	
4,18	$O_2 + H \rightarrow HO + O$		see reverse reaction	
4,18M	$O_2 + H + M \rightarrow HO_2 + M$ (f)			
20,M	$HO_2 + M \rightarrow O_2 + H + M$ (r)			
	†*This Survey	203-404	$k_f = 6.7 \times 10^{-33} \exp(290/T)$ $cm^6 molecule^{-2} s^{-1}$	±.07 (a)
			M = Ar or He, $k(300) = 1.8 \times 10^{-32}$	
			Rel. M efficiencies: Ar(1.0), He(1.0), N_2(3.1), O_2(3.1), H_2O(25)	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
			(a) This evaluation is based on the 300 K data reviewed by Baulch, et al (1972) and the recent studies by Hikida, et al (1971), Kurylo (1972) and Wong and Davis (1974).	
	Baulch, et al (1972) eval.	300-2000	$k_f = 4.1 \times 10^{-33} \exp(500/T)$ M = Ar	±.2
			Rel. M eff.: Ar(1.0), He(1.0), N_2(1.3), O_2(1.3), H_2O(21)	
			$k_r = k_f/K_{eq} = 3.5 \times 10^{-9} \exp(-23000/T)$ M = Ar	±0.2
	Bishop, Dorfman (1970)	300	$k_f = 2.35 \times 10^{-32}$ M = Ar	
	Hikida, Eyre, Dorfman (1971)	300	1.64×10^{-32} M = Ar	
	Ahumada, Michael, Osborne (1972)	300	0.75×10^{-32} M = He	
			Rel. M efficiencies: He(1.0), Ar(0.8)	
	Allen, Moortgat (1973)	115-300	$1.4(\pm 0.14) \times 10^{-33} \exp(+700(\pm 50)/T)$, M = Ar	
			Rel. M eff.: at 297K: Ar(1.0), He(0.97), H_2(1.28).	
	Kurylo (1972)	203-404	$6.7 \times 10^{-33} \exp(235/T)$	
			Rel. M eff.: Ar(1.0), He(1.0), N_2(3.4)	
	Wong, Davis (1974)	220-360	$6.8 \times 10^{-33} \exp(340/T)$	
			Rel. M efficiencies:	
			Ar(1.0), He(0.93) N_2(2.8), H_2(3.0), CH_4(21.5)	
	Westenberg, deHaas (1972a)	300	1.9×10^{-32} M = Ar or He	
	Slack (1977)	980-1176	$(9.1 \pm 1.6) \times 10^{-33}$ M = N_2	
		964-1075	$(6.1 \pm 1.1) \times 10^{-33}$ M = Ar	(a)
		200-2000	$1.85 \times 10^{-28} T^{-1.42}$ M = N_2	(b)
		200-2200	$5.8 \times 10^{-30} T^{-1}$ M = Ar	(b)
			(a) reanalysis of literature	
			(b) recommendation based on this work and data from literature	
4,21	$O_2 + H_2 \rightarrow H + HO_2$		see reverse reaction	
4,21	$O_2 + H_2 \rightarrow HO + HO$			
	Baulch, et al (1972) review		no recommendation	
4,22	$O_2 + H_2O \rightarrow HO_2 + HO$			
	Baulch, et al (1972) review		no recommendation	
4,23	$O_2 + H_2O_2 \rightarrow HO_2 + HO_2$			
	Baulch, et al (1972) review		no recommendation	
4,24	$O_2 + HNO \rightarrow NO + HO_2$			
	Demerjian, et al (1974) review	300	$< 2.1 \times 10^{-20}$, E/R > 5000K	estimated
4,27	$O_2 + SO \rightarrow SO_2 + O$		see reverse reaction	
4,31	$O_2 + HS \rightarrow SO + HO$			
	Cupitt, Glass (1974)	295	$< 10^{-13}$	
4,35M	$O_2 + Cl + M \rightarrow ClOO + M$ (f)			
37,M	$ClOO + M \rightarrow Cl + O_2 + M$ (r)			
	†NASA (1977) eval	200-300	$k_r = 5.8 \times 10^{-9} \exp(-3580/T)$	(+2, -1) (a)
			(a) $k_r = k_f/Keq$	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
	†Nicholas, Norrish (1968)	293	$k_f = 1.7 \times 10^{-33}$ $cm^6 molecule^{-2} s^{-1}$	
	Clyne and Coxon (1968)	300	$k_f = < 5.5 \times 10^{-33}$	
	Stedman (1968)	200-300	$k_f = 5.5 \times 10^{-34}$	(b)
	(b) As quoted by Clyne and Coxon (1968).			
4,46a	$O_2 + CN \rightarrow NCO + O$			
	Albers, et al (1975)	275-398	$5.3 \times 10^{-11} \exp(-500 \pm 170/T)$	
4,47	$O_2 + CHO \rightarrow CO + HO_2$			
	†*Washida, et al (1974)	297	$k/k(O + CHO) = 2.74 \pm 0.21 \times 10^{-2}$ yielding $k = 5.7 \pm 1.2 \times 10^{-12}$	
	Demerjian, et al (1974) review	300	1.7×10^{-13}	estimated
	Peeters, Mahnen (1973)	1400-1800	5×10^{-11}	
4,49	$O_2 + CH_3 \rightarrow CH_2O + HO$			
	Washida, Bayes (1976)	259-341	$2.9 \times 10^{-13} \exp(-940/T)$	
	Basco, et al (1972)	295	3×10^{-16}	estimated (a)
	a. Based on negative result and sensitivity limit. Other measurements at higher T suggest an appreciable activation energy.			
4,49M	$O_2 + CH_3(+M) \rightarrow CH_3O_2(+M)$			
	Laufer, Bass (1975)	298	$10^{12} \times k$ / $P(N_2)$/torr: 0.45 / 50; 0.7 / 100; 1.2 / 700	(a)
			1.7	(b)
	Washida, Bayes (1976)	300	5.0×10^{-13}	(b)
			1.9×10^{-31} $cm^6 molecule^{-2} s^{-1}$ $M = N_2$	(c)
	Hochanadel, et al (1977)	295	2.2×10^{-12}	(b)
	Basco, et al (1972)	295	5.1×10^{-13}	(b)
			2.6×10^{-31} $cm^6 molecule^{-2} s^{-1}$ $M = N_2$	(c)
	van den Bergh, Callear (1971)	295	1.8×10^{-12} preliminary	(b)
			6×10^{-31} $cm^6 molecule^{-2} s^{-1}$ $M = C_3H_8$ preliminary	(c)
	(a) Values are based on $k(CH_3 + CH_3) = 9.5 \times 10^{-11}$, given in Bass, Laufer (1973). (b) 2nd order high pressure limit. (c) 3rd order low pressure limit.			
4,50	$O_2 + CH_3O \rightarrow . . .$		see $CH_3O + O_2$	
5,M	$O_2(^1\Delta) + M \rightarrow O_2 + M$			
	*Hampson, et al (1973) review	285-322	$2.2 \times 10^{-18} (T/300)^{0.8}$ $M = O_2$	±0.1
	Huestis, et al (1974)	77	1.1×10^{-18} $M = O_2$	(a)
	(a) Liquid phase. When combined with gas phase data of Findlay and Snelling (1971a) (summarized in Hampson, et al (1973) $k = 2.2 \times 10^{-18} (T/300)^{0.5}$			

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
	*Hampson, et al (1973) review	300	$<2 \times 10^{-20}$ M = N_2	
	Collins, et al (1973)	300	1.4×10^{-19}, M = N_2	±0.06
	*Penzhorn, et al (1974)	300	3.9×10^{-20} M = SO_2	
		300	2.1×10^{-19} M = H_2S	
	Penzhorn, et al (1975)	300	$k \times 10^{18}$ / M: 0.4 / CF_2Cl_2 ≤0.08 / CCl_4 1.01 / CH_3Cl 0.87 / CH_2Cl_2 0.92 / $CHCl_3$	
	Breckenridge, Miller (1972)	300	$< 2 \times 10^{-15}$ M = SO_2	(a)
	Fisher, McCarty (1966)	300	$< 3 \times 10^{-16}$ M = CO	(a)
			(a) total rate, quenching and reaction	
5,7	$O_2(^1\Delta) + O_3 \rightarrow 2O_2 + O$			
	Clark, Jones, Wayne (1970)	195-439	$6.6 \times 10^{-13} \exp(-1560/T)$	±0.24
	Findlay, Snelling (1971)	283-321	$4.5 \times 10^{-11} \exp(-2830/T)$	±0.11
	Becker, et al (1972)	296-360	$6.0 \times 10^{-11} \exp(-2850/T)$	±0.17
	Collins, et al (1973)	300	4.4×10^{-15}	±0.11
	Schofield (1972) review	283-321	$4.5 \times 10^{-11} \exp(-2830/T)$	±0.11
5,8	$O_2(^1\Delta) + N \rightarrow NO + O$			
	Schmidt, Schiff (1973)	300	$k < k(N + O_2 \rightarrow NO + O)$	probably
	Westenberg, et al (1970)	195-300	$k << k(N + O_2 \rightarrow NO + O)$	
	Clark, Wayne (1970)	195-431	$k = 2 \times 10^{-14} \exp(-600/T)$	(a)
			(a) probably refers to physical deactivation, not chemical reaction; see above refs	
5,9	$O_2(^1\Delta) + NO \rightarrow O_2 + NO(v > 0)$			
	*Becker, et al (1971)	300	4.5×10^{-17}	±0.15
	Yaron, et al (1976)	300	2.5×10^{-17}	±0.1
	Ciachardi, et al (1976)	293	$(4.5 \pm 1) \times 10^{-17}$	
	Ogryzlo, Thrush (1973)	300	NO(v = 4) observed	
5,18	$O_2(^1\Delta) + H \rightarrow$ products			
	Schmidt, Schiff (1973)	300	$(2.5 \pm 0.5) \times 10^{-14}$	(a)
			(a) expt could not distinguish between chemical rxn and physical quenching	
	Westenberg, et al (1970)	300	rxn to give HO + O as products not observed	
5,27	$O_2(^1\Delta) + SO \rightarrow O_2 + SO(^1\Delta)$			
	Breckenridge, Miller (1972)	300	$3.5 \pm 0.36 \times 10^{-13}$	
6,M	$O_2(^1\Sigma) + M \rightarrow O_2 + M$			
	*Hampson, et al (1973) review	300	1.5×10^{-16}, M = O_2	±0.12
			2.0×10^{-15}, M = N_2	±0.1
			4×10^{-12}, M = H_2O	±0.18

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
7,hν	$O_3 + h\nu \rightarrow O(^3P) + O_2(^3\Sigma_g^-)$			
	*Hampson, et al (1973) review		ϕ = 1, 450< λ <750 nm - Chappuis bands ϕ = 0 250< λ <350 nm	
	Johnston (1973)		$k = 3.39 \times 10^{-4} s^{-1}$ (Daylight) (450< λ <750nm - Chappuis bands)	
7,hν	$O_3 + h\nu \rightarrow O(^3P) + O_2(^1\Delta$ or $^1\Sigma)$			
	*This survey		ϕ = 0, λ <303nm Total quantum yield ($O^3P + O^1D$) equals unity for 303< λ <350nm	
7,hν	$O_3 + h\nu \rightarrow O(^1D) + O_2(^1\Delta)$			
	†*Lin, DeMore (1973)		λ/nm — $\phi\ O(^1D)$ — λ/nm — $\phi\ O(^1D)$ — (a) ≤303 — 1.00 — 310 — 0.25 304 — 0.99 — 311 — 0.15 305 — 0.95 — 312 — 0.10 306 — 0.90 — 313 — 0.07 307 — 0.80 — 314 — 0.04 308 — 0.55 — 315 — 0.02 309 — 0.35 — ≥316 — 0 (a) As tabulated in review by Molina (1977) Relative values norm. to ϕ = 1 for λ <300nm	
	Hampson, et al (1973) review		See for discussion of earlier work	
7,hν	$O_3 + h\nu \rightarrow O(^1D) + O_2(^1\Sigma_g^+)$			
	*Hampson, et al (1973) review		ϕ = 0, 250< λ <350 nm	
7,M	$O_3 + M \rightarrow O + O_2 + M$		see reverse reaction	
7,8	$O_3 + N \rightarrow NO + O_2$			
	†*NASA (1977) eval	200-300	$2 \times 10^{-11} \exp(-1070/T)$ (a) Accepts room temp. rec. of Baulch "A factor" chosen; E_{act} derived	±0.3 at 230K
	Baulch, et al (1973) review	300	5.7×10^{-13}	±0.2
7,9	$O_3 + NO \rightarrow NO_2 + O_2$ (f)			
4,10	$O_2 + NO_2 \rightarrow NO + O_3$ (r)			
	†*NASA (1977) eval	200-300	$k_f = 2.1 \times 10^{-12} \exp(-1450/T)$ (a) based on results in Birks et al (1976). Lower "A factor" derived from reconsideration of primary data	±0.15 (a)
	Birks, et al (1976)	203-361	$k_f = 2.34 \pm 0.23 \times 10^{-12} \exp(-1450 \pm 50/T)$	
	Hampson, et al (1973) review	198-330	$k_f = 9 \times 10^{-13} \exp(-1200/T)\ cm^3 molecule^{-1} s^{-1}$	±0.11
	Stedman, Niki (1973)	298	$k_f = 1.73 \pm 0.1 \times 10^{-14}$	±0.2
	Baulch, et al (1973) review	200-350	$k_f = 1.5 \times 10^{-12} \exp(-1330/T)$	±0.2
		200-350	$k_r = k_f/K_{eq} = 2.8 \times 10^{-12} \exp(-25400/T)$	±0.2
	Ghormley, et al (1973)	298	$k_f = 1.41 \times 10^{-14}$	
	Bemand, et al (1974)	300	$k_f = 1.81 \pm 0.13 \times 10^{-14}$	
	Becker, Schurath, Seitz (1974)	290	$k_f = 1.70 \times 10^{-14}$	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
7,9	$O_3^* + NO \rightarrow NO_2^*(^2B_{1,2}) + O_2$ (1) $\rightarrow NO_2^*(^2A_1) + O_2$ (2) $\rightarrow O_3 + NO$ (3)			
	Kurylo, et al (1975)	153-373	see discussion	
	Bar-Ziv, Moy, Gordon (1978)	158-437	see discussion	
	Hui, Cool (1978)	138-410	$k_1 = 1.0 \times 10^{-12} \exp(-1450/T)$ $k_2 = 3.8 \times 10^{-13} \exp(-520/T)$ $k_3 = 1.1 \times 10^{-13}$ at 333 K and at 143 K with minimum value of 0.62×10^{-13} at approx. 230K Discussion Measured quantity in all studies is $(k_1 + k_2 + k_3)$. Values of this quantity measured by Kurylo et al and by Hui, Cool are in good agreement; values reported by Bar-Ziv, Moy and Gordon are systematically higher below 300K. Hui and Cool derived values as a function of temperature for k_1, k_2, and k_3 given above from an analysis of the temperature dependent data for $(k_1 + k_2 + k_3)$ reported by the three groups, the temperature dependence of the enhancement factor for rxn channel (1) reported by Moy, Bar-Ziv and Gordon (1977), their own temperature dependent data for the ratio of the enhancement factors for rxn channels (1) and (2) and the rate constant for channels (1) and (2) for thermal ozone reported by Clough and Thrush (1967)	
7,10 4,11	$O_3 + NO_2 \rightarrow NO_3 + O_2$ (f) $O_2 + NO_3 \rightarrow O_3 + NO_2$ (r)			
	†*NASA (1977) eval	220-340	$k_f = 1.2 \times 10^{-13} \exp(-2450/T)$	±0.1 (a)
	Davis, Prusazcyk, Dwyer, Kim (1974)	260-343	$k_f = 9.76 \pm 0.54 \times 10^{-14} \exp(-2427 \pm 140/T)$	
	Graham, Johnston (1974)	231-298	$k_f = 1.34 \pm 0.11 \times 10^{-13} \exp(-2466 \pm 30/T))$	
	Huie, Herron (1974a)	259-362	$k_f = 1.57 \pm 0.41 \times 10^{-13} \exp(-2509 \pm 76/T)$	
	Baulch, et al (1973) review	286-302	$k_f = 9.8 \times 10^{-12} \exp(-3500/T)$	±0.3 (b)
		300	$k_r = 7 \times 10^{-34}$ based on k_f	±0.3
	Wu, Morris, Niki (1973)	299	$k_f = 4.4 \times 10^{-17}$	±0.06 (c)
	Ghormley, et al (1973)	298	$k_f = 3.2 \times 10^{-17}$	±0.07
	Stedman, Niki (1973)	298	$k_f = 6.5 \pm 0.8 \times 10^{-17}$	
	Becker, Schurath, Seitz (1974)	289	$k_f = 3.24 \times 10^{-17}$	

(a) Derived by combining results from the three 1974 temperature dependent studies
(b) Based on Johnston, Yost (1949)
(c) Revision, based on later experiments, of value reported by Stedman and Niki (1973)

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
7,18	$O_3 + H \rightarrow HO + O_2$			
	*Clyne, Monkhouse (1977)	298-638	$1.0 \pm 0.2 \times 10^{-10} \exp(-516 \pm 60/T)$	±0.2 (a)
			(a) NASA (1977) evaluation selected preliminary value reported by these authors, $k = 1.2 \times 10^{-10} \exp(-560/T)$ with $\Delta \log k$ increased to ±0.3 at 230K.	
	Lee, et al (1978)	219-360	$1.3 \pm 0.3 \times 10^{-10} \exp(-449 \pm 58/T)$	
	Phillips, Schiff (1962)	300	$2.6 \pm 0.5 \times 10^{-11}$	(b)
			(b) Quoted by Hampson, et al (1973) review and Baulch, et al (1976) review	
7,19	$O_3 + HO \rightarrow HO_2 + O_2$			
	†*NASA (1977) eval	200-300	$1.5 \times 10^{-12} \exp(-1000/T)$	±0.3 (a)
			(a) Adjusted from recommendation in Hampson et al (1973) review because of error in derivation of O_3 conc. from absorption meas.	
	Hampson, et al (1973) review	220-450	$1.6 \times 10^{-12} \exp(-1000/T)$	±0.3
	Anderson, Kaufman (1973)	220-450	$1.3 \times 10^{-12} \exp(-956/T)$	
	Baulch, et al (1976) review	300	6.5×10^{-14}	±0.3
	DeMore (1973)	300	8×10^{-14}	
	DeMore (1975)	271-333	$k/k(OH + CO) = 16.8 \exp(-1230/T)$ at 700 torr CO_2	
	Davis (1976)	300	$7.5 \pm 0.3 \times 10^{-14}$	
	Kurylo (1973)	298	6.5×10^{-14}	±0.06
7,19	$O_3 + HO(v_1 > 0) \rightarrow$ products			
	Coltharp, Worley, Potter (1971)	300	$v_1(HO)$ — $10^{12} \times k(300\ K)$: CWP / SJ	
			2: 1.9±1.1	
			3: 2.4±0.9	
	Streit, Johnston (1976)		4: 2.8±0.8 / 3.7±0.1	
			5: 3.4±0.7 / 4.5±0.1	
			6: 5.3±0.6 / 7.1±0.2	
			7: 6.5±0.5 / 8.5±0.2	
			8: 6.7±0.5 / 8.9±0.2	
			9: 7.7±0.3 / 11 ±0.4	
7,20	$O_3 + HO_2 \rightarrow HO + 2O_2$			
	†*NASA (1977) eval.	200-300	$7.3 \times 10^{-14} \exp(-1275/T)$	±0.3
	Simonaitis, Heicklen (1973b)	225-298	$k/(k_{ref})^{0.5} = 1.9 \times 10^{-8} \exp(-1000/T)$	(a)
	DeMore, Tschuikow-Roux (1974)	273-332	$k/(k_{ref})^{0.5} = 1.1 \times 10^{-7} \exp(-1550 \pm 250/T)$	(a)
	Lloyd (1974) review	200-500	$1.7 \times 10^{-13} \exp(-1400/T)$	>±0.3
	Baulch, et al (1976) review	300	1.5×10^{-15}	±0.2
			(a) $k_{ref} = k(HO_2 + HO_2 \rightarrow H_2O_2 + O_2)$ Preferred value averages temp. dependence of these studies and is based on k_{ref} value given in this table.	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
7,27	$O_3 + SO \rightarrow O_2 + SO_2$			
	Schofield (1973) review	223-303	$2.5 \times 10^{-12} \exp(-1050/T)$	±0.5
	Baulch et al (1976) review		no recommendation	
7,28	$O_3 + SO_2 \rightarrow SO_3 + O_2$			
	Daubendiek, Calvert (1974)	300	$k < 8 \times 10^{-24}$	
	Davis, Prusazcyk, Dwyer, Kim (1974)	300	$k < 2 \times 10^{-22}$	
7,32	$O_3 + H_2S \rightarrow$ products			
	Glavas, Toby (1975)	298-343	$7 \times 10^{-14} \exp(-3400/T)$	±0.4
	Becker, Inocencio, Schurath (1975)	300	$< 2 \times 10^{-20}$	
7,35	$O_3 + Cl \rightarrow ClO + O_2$			
	†*Watson (1977) review	205-298	$2.7 \times 10^{-11} \exp(-257/T)$	±0.12 at 230K
	Clyne, Nip (1976)	221-629	$5.18 \times 10^{-11} \exp(-418/T)$	
	Kurylo, Braun (1976)	213-298	$2.72 \times 10^{-11} \exp(-298/T)$	
	Watson, et al (1976)	220-350	$3.08 \times 10^{-11} \exp(-290/T)$	
	Zahniser, et al (1976)	210-360	$2.17 \times 10^{-11} \exp(-171/T)$	
7,35Br	$O_3 + Br \rightarrow BrO + O_2$			
	†*Leu, DeMore (1977)	224-422	$3.34 \times 10^{-11} \exp(-978/T)$	±0.2 at 230K
7,36	$O_3 + ClO \rightarrow OClO + O_2$ (a) $\rightarrow ClOO + O_2$ (b)			
	†*NASA (1977) eval	200-300	$k_a = 1 \times 10^{-12} \exp(-4000/T)$ $k_b = 1 \times 10^{-12} \exp(-4000/T)$	+0.6, -2.0 at 230K (a)
	Watson (1977) review	300	$< 5 \times 10^{-15}$	
			(a) Based on unpublishd 300K results of Lin and DeMore. Branching ratio unknown - assumed equal to unity.	
7,36Br	$O_3 + BrO \rightarrow$ products			
	†*Clyne, Cruse (1970)	293	$k < 1 \times 10^{-14}$	upper limit only
7,45	$O_3 + CO \rightarrow CO_2 + O_2$			
	Arin, Warneck (1972)	296	$<4 \times 10^{-25}$	
7,48	$O_3 + CH_2O \rightarrow$ products			
	Braslavsky, Heicklen (1976)	300	$\leq 2 \times 10^{-24}$	±0.3 upper limit
7,49	$O_3 + CH_3 \rightarrow CH_3O + O_2$ (a) $\rightarrow CH_2O + HO_2$ (b)			
	Simonaitis, Heicklen (1975)	221-298	$(k_a + k_b)/k_{ref} = 12 \exp(-525/T)$ (a) k_{ref} is 2nd order high pressure limit for $CH_3 + O_2(+M) \rightarrow CH_3O_2(+M)$	(a)
7,51	$O_3 + CH_3O_2 \rightarrow$ products			
	Simonaitis, Heicklen (1975)	300	$<2.4 \times 10^{-17}$	
7,54	$O_3 + CH_3ONO \rightarrow$			
	Hastie, et al (1976)	298-325	$6.8 \times 10^{-13} \exp(-5315/T)$	
7,56	$O_3 + CH_4 \rightarrow$ products			
	Dillemuth, et al (1960)	310-340	$2.7 \times 10^{-13} \exp(-7700/T)$	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
7,57	$O_3 + C_2H_4 \rightarrow$ products			
	*Herron, Huie (1974)	235-362	$9.0 \times 10^{-15} \exp(-2560/T)$	±0.1
	Demerjian, et al (1974) review	300	2.7×10^{-18}	
	DeMore (1969)	178-233	$3.2 \times 10^{-15} \exp(-2400/T)$	
	Stedman, et al (1973)	300	$1.55 \pm 0.15 \times 10^{-18}$	
	Davis (1974)	300	$1.6 \pm 0.2 \times 10^{-18}$	
	Becker, Schurath, Seitz (1974)	280-360	$1.2 \times 10^{-14} \exp(-2490 \pm 100/T)$	
	Japar, Wu, Niki (1974)	298	$1.9 \pm 0.1 \times 10^{-18}$	
	Toby, et al (1976)	303	$1.7 \pm 0.1 \times 10^{-18}$	
7,59	$O_3 + C_3H_6 \rightarrow$ products			
	*Herron, Huie (1974)	235-362	$6.1 \times 10^{-15} \exp(-1900/T)$	±0.1
	Demerjian et al (1974) review	300	1.0×10^{-17}	
	DeMore (1969)	183, 193, 300	$1.6 \times 10^{-15} \exp(-1600/T)$	(a)
	Stedman, et al (1973)	300	$1.25 \pm 0.1 \times 10^{-17}$	
	Becker, Schurath, Seitz (1974)	280-360	$1.1 \times 10^{-14} \exp(-1970 \pm 100/T)$	
	Japar, Wu, Niki (1974)	298	1.30×10^{-17}	
			(a) Includes 300 K point of Hanst et al (1958).	
7,59	O_3 + allene → products			
	Toby, Toby (1975)	273-343	$1.6 \times 10^{-15} \exp(-2750/T)$ (a) Mechanism reconsidered. Data in Toby and Toby (1974a)	±0.7 (a)
7,59	O_3 + 1-butene → products			
	Huie, Herron (1975)	225-363	$2.9 \pm 0.2 \times 10^{-15} \exp(-1686 \pm 20/T)$	
	Japar, Wu, Niki (1974)	298	1.23×10^{-17}	
7,59	O_3 + cis-2-butene → products			
	Huie, Herron (1975)	225-363	$3.1 \pm 0.7 \times 10^{-15} \exp(-956 \pm 54/T)$	
	Japar, Wu, Niki (1974)	298	1.61×10^{-16}	
7,59	O_3 + trans-2-butene → products			
	Huie, Herron (1975)	225-363	$6.0 \pm 1.0 \times 10^{-15} \exp(-1051 \pm 43/T)$	
	Japar, Wu, Niki (1974)	298	2.60×10^{-16}	
7,59	O_3 + 1,3-butadiene → products			
	Toby, Toby (1975)	273-343	$1 \times 10^{-13} \exp(-2900/T)$	±0.5
	Becker, Schurath, Seitz (1974)	280-360	$5.4 \times 10^{-14} \exp(-2680/T)$	
7,64	O_3 + cis-$C_2Cl_2H_2$ → products			
	Blume et al (1976)	296	3.7×10^{-20}	
7,64	O_3 + trans-$C_2Cl_2H_2$ → products			
	Blume et al (1976)	296	2.5×10^{-19}	
8,8M	$N + N + M \rightarrow N_2 + M$			
	*Baulch, et al (1973) review	100-600	$8.3 \times 10^{-34} \exp(+500/T) cm^6 molecule^{-2} s^{-1}$ $M = N_2$	±0.2(200-600K) <0.2 (T<200K)
			where $-d[N]/dt = 2k[N]^2[M]$	
	Taylor (1975) review	2000-10000	$7.6 \times 10^{-32} T^{-1/2}$ $M = N_2$	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant† $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
			$3.0 \times 10^{-32} T^{-1/2}$ M = O_2, O, NO	
			$6.5 \times 10^{-27} T^{-3/2}$ M = N	
8,9	N + NO → N_2 + O (f)			
1,12	O + N_2 → N + NO (r)			
	†*Clyne, McDermid (1975)	298-670	$k_f = 8.2 \times 10^{-11} \exp(-410/T)$	±0.2 at 230K
	Baulch, et al (1973) review	300-5000	$k_f = 2.7 \times 10^{-11}$	±0.1 (a)
		2000-5000	$k_r = 1.3 \times 10^{-10} \exp(-38000/T)$	±0.3
			(a) Uncertainty increases to ±0.3 for T> 2000. k_f based on 300 K data and k_r(T> 2000).	
	Taylor (1975) review	2000-10000	$k_f = 2.7 \times 10^{-11}$	
8,10	N + NO_2 → N_2O + O			
	†*NASA (1977) eval.	200-300	$2 \times 10^{-11} \exp(-800/T)$	±0.3 at 230K (a,b)
	Clyne, McDermid (1975)	298	1.4×10^{-12}	
			(a) Accepts room temp. result of Clyne + McDermid "A factor" chosen; E_{act} derived	
			(b) Believed to be sole reaction channel	
8,19	N + HO → NO + H			
	*Baulch, et al (1973) review	300	5.3×10^{-11}	±0.3 (a)
			(a) Based on k/k(O + HO → O_2 + H) = 1.4	
8,27	N + SO → products			
	Baulch, et al (1976) review		no recommendation	
8,29	N + SO_3 → products			
	Baulch, et al (1976) review		no recommendation	
8,37	N + OClO → NO + ClO			
	Watson (1977) review	298	$k < 6 \times 10^{-13}$	preliminary value
9,hν	NO + hν			
	Hampson, et al (1973a) review		Recommended values of oscillator strengths from which absorption cross sections can be derived are given for β, γ, and ε bands. Recommended values of absorption cross section 106 < λ < 135 nm. No recommended quantum yield values.	
	*Bethke (1959)		Oscillator strength for δ bands, confirmed by Mandelman and Carrington (1974)	
9,M	NO + M → N + O + M			
	Baulch, et al (1973) review	4200-6700	Insufficient data for a reliable recommendation. Use, with caution: $6.6 \times 10^{-4} T^{-1.5} \exp(-75.5 \times 10^3/T)$ cm^3 $molecule^{-1} s^{-1}$ (M = Ar, O_2, N_2) k(M = NO, N, O)/k(Ar) ~ 18	
9,9	NO + NO → N + NO_2			
	Baulch, et al (1973) review		Endothermic. Unimportant compared to NO + NO → N_2O + O	
9,9	NO + NO → N_2O + O		see reverse reaction	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
9,9,4	$NO + NO + O_2 \rightarrow NO_2 + NO_2$		see $O_2 + NO + NO \rightarrow NO_2 + NO_2$	
9,10,22	$NO + NO_2 + H_2O \rightarrow 2HNO_2$ (f) $2HNO_2 \rightarrow NO + NO_2 + H_2O$ (r)			
	*Chan, et al (1976)	296	$k_f = 6.0 \times 10^{-38} cm^6 molecule^{-2} s^{-1}$ $k_r = 9.5 \times 10^{-19} cm^3 molecule^{-1} s^{-1}$	
	Hampson, et al (1973) review	300	Reviewed earlier work, probably heterogeneous	
9,11	$NO + NO_3 \rightarrow 2NO_2$			
	Graham, Johnston (1978)	300	$(1.9 \pm 0.4) \times 10^{-11}$	
	Baulch, et al (1973) review	300	$\sim 2 \times 10^{-11}$	±0.7 estimated
	Johnston (1966) review	300	8.3×10^{-12} Temperature effect is probably zero or very small.	
9,15	$NO + NH \rightarrow$ products			
	Hansen, et al (1976)	300	4.7×10^{-11}	±0.1
	Gordon, et al (1971)	300	3.8×10^{-11}	
	Mulvihill, Phillips (1975)	1500	$N_2 + O + H$ identified as products of major rxn channel	
9,16	$NO + NH_2 \rightarrow N_2 + H_2O$*			
	*Hancock, et al (1975)	298	2.1×10^{-11}	
	Lesclaux, et al (1975)	300	1.8×10^{-11} (a) $T^{-1.25}$ dependence observed 300-500K	(a)
	Gehring, et al (1973)	300	8×10^{-12}	±0.1
	Gordon, et al (1971)	300	2.7×10^{-11}	
9,18M	$NO + H + M \rightarrow HNO + M$			
	*This survey	220-400	$2.1 \times 10^{-32} \exp(300/T)$	±0.2
	Baulch, et al (1973) review	230-700	$1.5 \times 10^{-32} \exp(300/T)$ $cm^6 molecule^{-2} s^{-1}$ M = H_2	±0.2
	Atkinson, Cvetanovic (1973)	286-390	$2.5 \times 10^{-32} \exp(270/T)$ M = H_2	
	Allen, Moortgat (1973)	180-300	$5.6(\pm 0.6) \times 10^{-33} \exp(+375(\pm 65)/T)$, M = Ar	
	Thrush (1973) review	230-700	$2 \times 10^{-32} \exp(+300/T)$, M = H_2	
9,19	$NO + HO \rightarrow NO_2 + H$			
	Baulch, et al (1973) review	298-633	$5.2 \times 10^{-12} \exp(-15.1 \times 10^3/T)$ based on $k = 5.8 \times 10^{-10} \exp(-740/T)$ for reverse reaction (a) corrected expression	±0.2 (298K) (a) increasing to ±0.3(633K)
9,19M	$NO + HO(+M) \rightarrow HNO_2(+M)$			
	Hampson, et al (1973a) review		Elevation/km — k(T,M)	
		217	15 — 2.4×10^{-12}	Abs. value of log k ± 0.5
		217	20 — 1.5×10^{-12}	Relative value of k
		222	25 — 8.9×10^{-13}	at different altitudes
		227	30 — 4.8×10^{-13}	reliable to ± 20%
		237	35 — 2.6×10^{-13}	M = N_2
		251	40 — 1.1×10^{-13}	
		265	45 — 5.9×10^{-14}	
	Baulch, et al (1973) review	273-395	$2.2 \times 10^{-32} \exp(+1110/T)$ $cm^6 molecule^{-2} s^{-1}$ (3rd order low pressure limit)	M=He ±0.2 at 300K inc. to ±0.3 at 395K

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
		300	2×10^{-12} $cm^3 molecule^{-1} s^{-1}$ (2d order high pressure limit)	±0.3
	Anderson, et al (1974)	295,439	$5.8 \pm 1.2 \times 10^{-31} \times (295/T)^{+2.4}$ $cm^6 molecule^{-2} s^{-1}$ $M = N_2$ (3rd order low pressure limit) Relative efficiencies: N_2(1.0), Ar(0.58), He(0.57)	
	Howard, Evenson (1974)	296	$7.8 \pm 1.2 \times 10^{-31}$ $cm^6 molecule^{-2} s^{-1}$ $M = N_2$ (3rd order low pressure limit) Relative efficiencies: N_2(1.0), Ar(0.56), He(0.51)	
	Cox (1974a)	294	$k/k(H\dot{O} + C\dot{O}) = 40 \pm 7$ $k = 1.2 \times 10^{-11}$ $cm^3 molecule^{-1} s^{-1}$ (a) 2nd order rate constant, [M] = 1 atm $N_2 + \dot{O}_2$; $k_{ref} = 3 \times 10^{-13}$, this survey	(a)
	Harris, Wayne (1975)	300	$7 \pm 2 \times 10^{-31}$ $cm^6 molecule^{-2} s^{-1}$, M = Ar $15 \pm 5 \times 10^{-31}$, M = N_2 (3rd order low pressure limits)	
	Gordon, Mulac (1975)	435	$7.5 \pm 0.3 \times 10^{-12}$ $cm^3 molecule^{-1} s^{-1}$ (2nd order rate constant at 1 atm. $H_2\dot{O}$ vapor)	
	Atkinson, Hansen, Pitts (1975a)	298	$4.94 \pm 0.5 \times 10^{-13}$ M = 25 Torr N_2 (b) also data for M = Ar at 25-655 torr	(b)
	Cox, Derwent, Holt (1976)	298	1.17×10^{-11} M = 1 atm $N_2 + \dot{O}_2$ (c) relative to $k(H\dot{O} + H_2) = 7 \times 10^{-15}$	(c)
	Overend, et al (1976)	295	$0.956 \pm 0.05 \times 10^{-12}$ M = 25 torr N_2 $6.89 \pm 0.68 \times 10^{-12}$ M = 770 torr N_2	
	Sie, et al (1976b)	298	$k/k_{ref} = 16.1$ at 95 torr and = 22 at 408 and 768 torr total pressure, mostly H_2 where ref rxn is $H\dot{O} + C\dot{O} \rightarrow C\dot{O}_2 + H$	
9,20	$N\dot{O} + H\dot{O}_2 \rightarrow N\dot{O}_2 + H\dot{O}$			
	†*Howard, Evenson (1977)	296	$(8.1 \pm 1.5) \times 10^{-12}$	±0.4 at 230K
	Hack, et al (1975)	298-670	$2.0 \times 10^{-11} \exp(-1200/T)$	
	Simonaitis, Heicklen (1978)	245-328	$k/(k_{ref})^{0.5} = 6.4 \times 10^{-6} \exp(-700/T)$ (a) ref rxn: $2H\dot{O}_2 \rightarrow H_2\dot{O}_2 + \dot{O}_2$	(a)
	Cox, Derwent (1975)	296	1.2×10^{-12}	
	Payne, Stief, Davis (1973)	300	3×10^{-13}	±0.5
	Glanzer, Troe (1975)	1350-1700	7.5×10^{-12}	±0.5
9,20M	$N\dot{O} + H\dot{O}_2(+M) \rightarrow HN\dot{O}_3(+M)$			
	Cox, Derwent (1975)	296	1.4×10^{-13} at 1 atm $N_2 + \dot{O}_2$	
	Simonaitis, Heicklen (1976a)	296	$< 2 \times 10^{-15}$	
9,21	$N\dot{O} + H_2 \rightarrow HN\dot{O} + H$			
	Baulch, et al (1973) review	2000	5.3×10^{-18} cm^3 $molecule^{-1} s^{-1}$ (a) No data. Value based on reverse rate	±0.3 (a)

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
9,22	$NO + H_2O \rightarrow HNO + HO$			
	Baulch, et al (1973) review	2000	4×10^{-18}	±0.2 (a)
			(a) No data. Value based on reverse rate. (corrected)	
9,23	$NO + H_2O_2 \rightarrow HO + HNO_2$			
	*Hampson, et al (1973) review	300	$< 5 \times 10^{-20}$	
		500	$\sim 2 \times 10^{-20}$	
	Gray, et al (1972)	300	$< 5 \times 10^{-20}$	
9,35M	$NO + Cl + M \rightarrow ClNO + M$			
	†*NASA (1977) eval	200-300	$1.7 \times 10^{-32} \exp(+530/T)$ $M = N_2$	±0.6 at 230K (a)
			(a) see Watson (1977) review	
9,36	$NO + ClO \rightarrow NO_2 + Cl$			
	†*NASA (1977) eval	200-300	$1.0 \times 10^{-11} \exp(200 \pm 100/T)$	±0.3 at 230K
	Watson (1977) review	220-298	$8 \times 10^{-12} \exp(250/T)$	±0.1
	Zahniser, Kaufman (1977)	230-298	$k/k_{ref} = (0.52 \pm 0.05) \exp(373 \pm 23/T)$	(a)
			(a) $k_{ref} = k(Cl + O_3)$	
9,36Br	$NO + BrO \rightarrow NO_2 + Br$			
	†*NASA (1977) eval	200-300	2.1×10^{-11}	±0.4 at 230K
	Clyne, Watson (1975)	298	2.2×10^{-11}	±0.1
9,37	$NO + OClO \rightarrow NO_2 + ClO$			
	†*NASA (1977) eval	200-300	$2.5 \times 10^{-12} \exp(-600/T)$	±0.6 at 230K (a)
	Bemand, Clyne, Watson (1973)	300	3.4×10^{-13}	
			(a) Based on room temp. value of Bemand, Clyne, Watson; temp dependence estimated	
9,49M	$NO + CH_3 (+M) \rightarrow CH_3NO (+M)$			
	Laufer, Bass (1975)	298	$10^{11} \times k$ / $P(N_2)$/torr: .3 / 50; .45 / 100; 1.1 / 700	(a)
	Basco, et al (1970)	298	4×10^{-12}	(b)
	van den Bergh, Callear (1971)	295	1.7×10^{-11}	(b)
			(a) Values are based on $k(CH_3 + CH_3) = 9.5 \times 10^{-11}$ given in Bass, Laufer (1973).	
			(b) 2nd order high pressure limit.	
9,50	$NO + CH_3O \rightarrow$ . . .		see $CH_3O + NO \rightarrow$ . . .	
9,51	$NO + CH_3O_2 \rightarrow CH_3O_2NO$ (a) $\rightarrow CH_2O + HONO$ (b) $\rightarrow CH_3O + NO_2$ (c)			
	†Demerjian, et al (1974) review	300	$k_c = 3.3 \times 10^{-12} \exp(-500/T)$	estimate
	Cox, et al (1976)	298	$k_c \geq 1.2 \times 10^{-12}$	lower limit (a)
			(a) based on value of $k(CH_3O_2 + CH_3O_2)$	
	Pate, Finlayson, Pitts (1974)	296	Reaction proceeds exclusively through channel (c)	
	Simonaitis, Heicklen (1974)	298	$k_c/k = 0.80 \pm 0.15$ $(k = k_a + k_b + k_c)$	

No.	Reaction/Reference * = Preferred Value + = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
10,hν	$NO_2 + h\nu \rightarrow NO + O$			
	*Bayes (1974)		λ/nm: $\Phi(O(^3P))$ 295-398: $1.0 - 0.0008(\lambda - 275)$ 398: 0.90 ± 0.05 400: 0.76 ± 0.04 405: 0.37 ± 0.02 410: 0.14 ± 0.01	(a)
			(a) Based on analysis of data in Jones and Bayes (1973)	
	*Bass, Ledford, Laufer (1976)	235-298	Extinction coefficient values tabulated for λ = 185-410nm at 0.125nm intervals. Also gives values for N_2O_4	
10,M	$NO_2 + M \rightarrow NO + O + M$		see reverse reaction	
10,10	$NO_2 + NO_2 \rightarrow NO + NO_3$			
	Baulch, et al (1973) review		No recommendation	
10,10	$NO_2 + NO_2 \rightarrow NO + NO + O_2$			
	Baulch, et al (1973) review	600-2000	$3.3 \times 10^{-12} \exp(-13540/T)$ $k_1[NO_2]^2 = -(1/2)d[NO_2]/dt$	±0.15 (600-1000K) increasing to 0.3 at 2000K
10,10M	$NO_2 + NO_2 + M \rightarrow N_2O_4 + M$ (f) $N_2O_4 + M \rightarrow NO_2 + NO_2 + M$ (r)			
	Baulch, et al (1973) review	250-350	$k_f = 3.0 \times 10^{-35} \exp(1040/T) cm^6 molecule^{-2} s^{-1}$ (a) corrected expression; $k_f = k_r k_{eq}$	M = N_2 ±0.15(a)
	Baulch, et al (1973) review	250-350	$k_r = 4.2 \times 10^{-7} \exp(-5550/T)$	M = N_2 ±0.15
	Schofield (1973) review	250-350	$k_r = 3.3 \times 10^{-7} \exp(-5540/T)$	M = N_2 ±0.15
10,11 4,9,10	$NO_2 + NO_3 \rightarrow NO_2 + O_2 + NO$ (f) $O_2 + NO + NO_2 \rightarrow NO_2 + NO_3$ (r)			
	*Baulch, et al (1973) review	300-850	$k_f = 2.3 \times 10^{-13} \exp(-1000/T)$	±0.4 (a)
		300-500	$k_r = k_f/K_{eq} = 8 \times 10^{-41} \exp(400/T) cm^6 molecule^{-2} s^{-1}$	±0.4
	Graham, Johnston (1978)	338-396	$k_f = 2.5 \times 10^{-14} \exp(-1230/T)$ (a) Based on $N_2O_5 + M \rightarrow NO_2 + NO_3 + M$ and $2NO_2 \rightarrow 2NO + O_2$	
10,11M	$NO_2 + NO_3 (+M) \rightarrow N_2O_5 (+M)$			
	This survey		Elevation/km: k (T,M) $cm^3 molecule^{-1} s^{-1}$: Log (M)	
		217	15: 1.9×10^{-12}: 18.60	
		217	20: 1.1×10^{-12}: 18.27	
		222	25: 6.6×10^{-13}: 17.93	
		227	30: 4.5×10^{-13}: 17.58	
		237	35: 2.7×10^{-13}: 17.26	
		251	40: 1.5×10^{-13}: 16.92	
		265	45: 7.1×10^{-14}: 16.60	
10,11M 14,M	$NO_2 + NO_3 + M \rightarrow N_2O_5 + M$ (f) $N_2O_5 + M \rightarrow NO_2 + NO_3 + M$ (r)			

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
		300	$k_f = 3.8 \times 10^{-12}$ $cm^3 molecule^{-1} s^{-1}$ (2d order high pressure limit)	±0.4 (a)
		300-340	$k_r = 2.2 \times 10^{-5} \exp(-9700/T)$ $cm^3 molecule^{-1} s^{-1}$	±0.3 (a)
		273-300	$k_r = 5.7 \times 10^{14} \exp(-10600/T)$ s^{-1} (limiting first order expression)	±0.4 (a)
	Graham, Johnston (1978)	298-329	$K_{eq} = 1.2 \times 10^{-27} \exp(+11180/T) cm^3 molecule^{-1}$	
		273-300	$k_f(M) = 1.48 \times 10^{-13} \exp(+861/T) cm^3 molecule^{-1} s^{-1}$	(b)
			$k_r(M) = 1.24 \times 10^{14} \exp(-10317/T) s^{-1}$	(c)
			(a) $k_f = K_{eq} k_r$. $M = N_2O_5 + NO$ (b) 2d order rate const at 1 atm (c) 1st order rate const at 1 atm	
10,16	$NO_2 + NH_2 \rightarrow$ products			
	Jayanty, et al (1975d)	300	$k > k(NO + NH_2)$	
10,17	$NO_2 + NH_3 \rightarrow NH_2 + HNO_2$			
	Bedford, Thomas (1972)	615-660	$6.7 \times 10^{-12} \exp(-13900/T)$	
10,18	$NO_2 + H \rightarrow HO + NO$			
	Wagner, et al (1976a)	243-461	$7.1 \times 10^{-10} \exp(-505 \pm 84/T)$	±0.1
	Clyne, Monkhouse (1977)	298-653	$4.80 \times 10^{-10} \exp(-400 \pm 70/T)$	±0.1
	Bemand, Clyne (1977)	298	$1.13 \pm 0.22 \times 10^{-10}$	
10,19M	$NO_2 + HO + M \rightarrow HNO_3 + M$ (f)			
26,M	$HNO_3 + M \rightarrow HO + NO_2 + M$ (r)			
	†*NASA (1977) eval	200-350	$\log_{10}(k_f) = -AT/(B + T) - 0.5 \log_{10}(T/280)$ $A = A_1 + A_2 Z + A_3 Z^2 + A_4 Z^3$ $B = B_1 + B_2 Z + B_3 Z^2$ $A_1 = 31.62273$ $B_1 = -327.372$ $A_2 = -0.258304$ $B_2 = 44.5586$ $A_3 = -0.0889287$ $B_3 = -1.38092$ $A_4 = 2.520173 \times 10^{-3}$ where $Z = \log_{10}[N_2]$ and is applicable only for the ranges $200 < T/K < 350$ and $16.3 < \log_{10}([N_2]/molecule\ .cm^{-3}) < 19.5$, with an estimated reliability in log k of ±0.10 (reliability analogous to 1σ). Air is approximately 6 percent less efficient than nitrogen as a third body; i.e., k for (M = Air) = 0.94 k for $M = N_2$ For normal tropospheric conditions of 1 atm air and T = 300K, above expression yields value of $k_f = 1.1 \times 10^{-11}$	
	Anastasi, Smith (1976)	296	$k_f = 2.6 \times 10^{-30}$ $M = N_2$ Rel. Efficiencies: N_2(1.0), He(0.34), Ar(0.42), O_2(0.68), SF_6(2.5)	
		220-550	n = -2.6 for temp dependence of form T^n, $M = N_2$ values given for bimolecular rate constant over	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
			ranges T = 220-550K and $[N_2] = 3 \times 10^{17}$ to 1.6×10^{19} molecule cm^{-3}	
	Baulch, et al (1973) review	273-400	$k_f = 3.6 \times 10^{-32} \exp(+1100/T) cm^6 molecule^{-2} s^{-1}$ M = He	±0.2
		800-1200	$k_r = 2.7 \times 10^{-9} \exp(-15400/T) cm^3 molecule^{-1} s^{-1}$ M = Ar	±0.4
		300	$k_f = 8 \times 10^{-12} cm^3 molecule^{-1} s^{-1}$ (2d order high pressure limit)	±0.4
	Anderson, et al. (1974)	295-450	$k_f = 2.3 \pm 0.5 \times 10^{-30} \times (295/T)^{+2.5} cm^6 molecule^{-2} s^{-1}$ M = N_2 Relative efficiencies: N_2(1.0), Ar(0.43), He(0.43)	
	Howard, Evenson (1974)	296	$k_f = 2.9 \pm 0.4 \times 10^{-30}$ M = N_2	
	Gordon, Mulac (1975)	435	$k_f = 5.3 \times 10^{-12} cm^3 molecule^{-1} s^{-1}$ (2nd order rate constant at 1 atm. H_2O vapor)	
	Harris, Wayne (1975)	300	$15 \pm 5 \times 10^{-31} cm^6 molecule^{-2} s^{-1}$, M = Ar $26 \pm 10 \times 10^{-31}$, M = N_2	
	Atkinson, Perry, Pitts (1976)	298	$k_f = (1.0 \pm 0.1) \times 10^{-30}$ M = Ar Values given for bimolecular rate constant over pressure range 25-646 torr Ar	
10,20M	$NO_2 + HO_2 + M \rightarrow HO_2NO_2 + M$			
	†*NASA (1977) eval	200-300	tentatively, use expression given for rxn 10,36M $NO_2 + ClO + M \rightarrow NO_2ClO + M$ with twice the assigned uncertainty	
	Simonaitis, Heicklen (1978)	245	$k[M]/k(HO_2 + NO) = 0.61$	(a)
		295	$k[M]/k(HO_2 + NO) = 0.036$	(a)
			(a) M = 700 torr H_2. Rxn to give $HONO + O_2$ is negligible	
	Howard (1977)	300	$(2.09 \pm 0.52) \times 10^{-31}$ M = N_2 Rel. eff: N_2(1.0), He(0.48); O_2(0.72); NO_2(3.2) $k(HO_2 + NO_2 \rightarrow HONO + O_2) < 3 \times 10^{-15}$	
	Cox, Derwent (1975)	298	$k[M] = 1.2 \times 10^{-13}$ for [M] = 1 atm product probably HO_2NO_2 not $HONO + O_2$ as assumed by authors	
10,28	$NO_2 + SO_2 \rightarrow SO_3 + NO$			
	Davis (1974)	300	$k < 2 \times 10^{-24}$	
10,35M	$NO_2 + Cl + M \rightarrow NO_2Cl + M$			
	†*Clyne, White (1974)	298	$7.2 \times 10^{-31} cm^6 molecule^{-2} s^{-1}$	±0.6 at 230K
10,36M	$NO_2 + ClO + M \rightarrow ClONO_2 + M$			
	†*NASA (1977) eval	200-300	$\frac{3.3 \times 10^{-23} T^{-3.34}}{1 + 8.7 \times 10^{-9} T^{-0.6} [M]^{0.5}}$ M = N_2 (a) Expression developed by Zahniser, Chang, Kaufman (1977)	+0.3, -0.1 at 230K (a)
	Birks, et al (1977)	250-356	$(4.40 \pm 0.66) \times 10^{-33} \exp(1087/T)$ M = N_2	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
		297	$9.57 \pm 0.28 \times 10^{-32}$ M = He	
	Leu, Lin, DeMore (1977)	298-417	$(3.69 \pm 0.24) \times 10^{-33} \exp(1150/T)$ M = N_2	
		248-417	$(2.66 \pm 0.35) \times 10^{-33} \exp(1140/T)$ M = He	
	Zahniser, Chang, Kaufman (1977)	251-365	$(3.54 \pm 0.06) \times 10^{-33} \exp(950/T)$ M = He	(a)
		251-365	$5.53 \times 10^{-24} T^{-3.15}$ M = He	
		297	1.52×10^{-31} M = N_2	
			(a) Two forms of temp dependence are given: $\exp(B/T)$ and T^{-n}	
10,49	$NO_2 + CH_3 \rightarrow CH_3O + NO$			
	Glanzer, Troe (1973) review	300-1400	3.3×10^{-11}	±0.25 (a)
			(a) Based on $k/k(CH_3 + NO) = 3.3$ at room temperature and on shock wave pyrolysis of CH_3NO_2	
10,49M	$NO_2 + CH_3 (+M) \rightarrow CH_3NO_2 (+M)$			
	Glanzer, Troe (1973) review	295	2.8×10^{-11} $cm^3 molecule^{-1} s^{-1}$	±0.1 (a)
			(a) Based on high pressure limit rate ratio $k/k(CH_3 + NO) = 1.7$	
10,49M	$NO_2 + CH_3 + M \rightarrow CH_3NO_2 + M$			
	Glanzer, Troe (1973) review	900-1400	6.9×10^{-31} $cm^6 molecule^{-2} s^{-1}$, M = Ar	(a)
			(a) $k_f = k_r K_{eq}$	
10,50	$NO_2 + CH_3O \rightarrow . . .$		see $CH_3O + NO_2 \rightarrow . . .$	
10,51	$NO_2 + CH_3O_2 \rightarrow CH_3O_2NO_2$ (a) $\rightarrow CH_2O + HONO_2$ (b) $\rightarrow CH_3O + NO_3$ (c)			
	*Heicklen (1973) review	298	$k_a/k = 0.75 \pm 0.05$ $k_b/k = 0.25 \pm 0.1$ $k_c/k < 0.1$	
11,hν	$NO_3 + h\nu \rightarrow NO_2 + O$ (1) $\rightarrow NO + O_2$ (2)			
	Graham, Johnston (1978)	300	table of absorption cross sections for wavelength region 400-700nm	(a)
			$j_1 = 0.099\ s^{-1}$	(b)
			$j_2 = 0.04\ s^{-1}$	(b)
			(a) This table also given in Molina's review (1977). Values supersede results in Johnston, Graham (1974)	
			(b) Specific photodissociation rates for troposphere with overhead sun.	
11,M	$NO_3 + M \rightarrow NO_2 + O + M$		see reverse reaction	
11,11	$NO_3 + NO_3 \rightarrow 2NO_2 + O_2$			
	Graham, Johnston (1978)	298-329	$8.5 \times 10^{-13} \exp(-2450/T)$	
	Baulch, et al (1973) review	293-309	$5 \times 10^{-12} \exp(-3000/T)$	±0.5 (a)
			(a) $-d[NO_3]/dt = 2k[NO_3]^2$. Based on rate of O_3 decomp. in presence of N_2O_5	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
11,22	$NO_3 + H_2O \rightarrow HNO_3 + HO$			
	Baulch, et al (1973) review	300	2.3×10^{-26} (a) $k_f = k_r K_{eq}$	±0.3 (a)
11,28	$NO_3 + SO_2 \rightarrow NO_2 + SO_3$			
	Daubendiek, Calvert (1975)	300	$k < ? \times 10^{-21}$	
	Davis (1976)	300	$k < 1 \times 10^{-21}$	preliminary
12,M	$N_2 + M \rightarrow N + N + M$			
	*Baulch, et al (1973) review	6000-15000	$6.1 \times 10^{-3} T^{-1.6} \exp(-113{,}200/T) cm^3 molecule^{-1} s^{-1}$ $M = N_2$	±0.5
12,19	$N_2 + HO \rightarrow N_2O + H$			
	*Baulch, et al (1973) review	700-2500	$5.4 \times 10^{-12} \exp(-40.4 \times 10^3/T)$ (a) $k_f = k_r K_{eq}$ (corrected expression)	±0.2 (a)
13,hν	$N_2O + h\nu \rightarrow$ products			
	Johnston, Selwyn (1975)	294	figures of absorption cross section vs λ for λ = 210-328nm. Negligible absorption for λ>260nm	
	Selwyn, et al (1977)	194-302	Absorption cross section values tabulated for λ = 173-240nm at 1 nm intervals for T = 194, 225, 243, 265 and 302K	
13,M	$N_2O + M \rightarrow N_2 + O + M$		see reverse reaction	
13,18	$N_2O + H \rightarrow N_2 + HO$			
	Albers, et al (1975)	718-1111	$(3.6 \pm 1.2) \times 10^{-10} \exp(-8710 \pm 350/T)$	
	Baulch, et al (1973) review	700-2500	$1.26 \times 10^{-10} \exp(-7600/T)$	±0.2
	Baldwin, et al (1973)	773	4.3×10^{-15}	±0.15
13,19	$N_2O + HO \rightarrow$ products			
	Chang, Kaufman (1977)	480	$< 4 \times 10^{-16}$	upper limit only
	Bierman, et al (1976)	298	$3.8 \pm 1.2 \times 10^{-17}$	
	Atkinson, Perry, Pitts (1976)	298	$< 2 \times 10^{-16}$	
		443	$< 2 \times 10^{-16}$	
	Gordon, Mulac (1975)	440	$< 2 \times 10^{-14}$	
13,36	$N_2O + ClO \rightarrow$ products			
	†*NASA (1977) eval	200-300	$k \leq 1 \times 10^{-12} \exp(-4260/T)$ (a) "A factor" chosen. E_{act} fitted to upper limit at T = 587K reported in Watson's review (1977)	±2 at 230K (a)
13,45	$N_2O + CO \rightarrow$ products			
	Milks, Matula (1973)	1169-1655	$3.5 \times 10^{-13} \exp(-8650/T)$	
14,hν	$N_2O_5 + h\nu \rightarrow . . .$			
	Molina (1977) review		table of absorption cross sections for wavelength range 206-380nm (a) Gives values for λ = 205-310nm from Graham, Johnston (1977) which supersede results in Johnston, Graham (1974). Also gives values for λ = 320-380nm from Jones, Wulf (1937)	(a)

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
	Murphy (1969)		0.5 x $\phi(-N_2O_5)$ = $\phi(O)$ = 0.31 λ = 280 nm Meas. by Holmes, Daniels (1934) are consistent	
	Hampson, et al (1973a) review		Survey of photochemistry	
	Daubendiek, Calvert (1974)		Figure giving molar extinction coefficient vs λ. 250 < λ/nm < 350	
14,M	N_2O_5 (+M) → NO_2 + NO_3 (+M)		Elevation/km k/s^{-1}	
	*This survey	217	15 5.0×10^{-7}	±0.5
		217	20 1.8×10^{-7}	
		222	25 3.0×10^{-7}	
		227	30 5.5×10^{-7}	
		237	35 1.9×10^{-6}	
		251	40 1.6×10^{-5}	
		265	45 4.4×10^{-5}	
			Extrapolated from data taken between 273 and 353 K.	
14,M	N_2O_5 + M → NO_2 + NO_3 + M		see reverse reaction	
14,22	N_2O_5 + H_2O → $2HNO_3$			
	Hampson, et al (1973) review	300	$k < 1 \times 10^{-20}$	
	Morris, Niki (1973)	298	$< 1.3 \times 10^{-20}$	
14,28	N_2O_5 + SO_2 → products			
	Daubendiek, Calvert (1974)	300	$k < 4 \times 10^{-23}$	
	Davis (1974)	300	$k < 8 \times 10^{-24}$	
16,18M	NH_2 + H + M → NH_3 + M			
	Baulch, et al (1973) review	2000-3000	$1.2 \times 10^{-33} \exp(11200/T)$ cm^6 $molecule^{-2} s^{-1}$, M = Ar ±0.3 (a) (a) $k_f = K_{eq} k_r$	
16,19	NH_2 + HO → NH_3 + O		see reverse reaction	
16,21	NH_2 + H_2 → NH_3 + H			
	Baulch, et al (1973) review	800	$< 10^{-16}$ $k_f = K_{eq} k_r$	approximate
16,22	NH_2 + H_2O → NH_3 + HO			
	Baulch, et al (1973) review		no data, no recommendation	
17,M	NH_3 + M → NH_2 + H + M			
	Baulch, et al (1973) review	2000-3000	$k = 1.5 \times 10^{-8} \exp(-42400/T)$ (M = Ar) (a) To be used when P(M) < 4 atm.	±0.3 (a)
17,18	NH_3 + H → NH_2 + H_2			
	Baulch, et al (1973) review	800	$< 10^{-16}$	approximate
17,19	NH_3 + HO → NH_2 + H_2O			
	*Smith, Zellner (1975)	228-472	$2.3 \times 10^{-12} \exp(-800/T)$	±0.1
	Perry, Atkinson, Pitts (1976a)	298-427	$2.93 \times 10^{-12} \exp(-860 \pm 150/T)$	
	Davis (1977)	300	$(1.4 \pm 0.1) \times 10^{-13}$	preliminary
	Cox, Derwent, Holt (1975)	300	$(1.2 \pm 0.4) \times 10^{-13}$	
	Hack, et al (1974)	298-669	$5.3 \pm 0.8 \times 10^{-12} \exp(-920/T)$	
	Stuhl (1973a)	298	1.5×10^{-13}	±0.1
	Kurylo (1973)	298	4.1×10^{-14}	±0.06
	Gordon, Mulac (1975)	418	$4.3 \pm 0.5 \times 10^{-13}$	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
17,36	$NH_3 + ClO \rightarrow$ products			
	Walker (1972)	670	$k < 5 \times 10^{-16}$ (a) As quoted by Watson (1977) review.	(a)
17a,18	$N_2H_4 + H \rightarrow H_2 + N_2H_3$			
	Stief, Payne (1976)	228-400	$(9.87 \pm 1.17) \times 10^{-12} \exp(-1200 \pm 50/T)$	
18,18M	$H + H + M \rightarrow H_2 + M$ (f)			
21,M	$H_2 + M \rightarrow H + H + M$ (r)			
	Baulch, et al (1972) review	300	$k_f = 8.3 \times 10^{-33}$ $cm^6 molecule^{-2} s^{-1}$ M = H_2	±0.2
		1700-5000	$= 1.8 \times 10^{-30} T^{-1}$ M = Ar Rel. efficiencies: H_2(1.0), Ar(0.25) $-d[H]/dt = 2k[H]^2[M]$	±0.3
		2500-5000	$k_r = 3.7 \times 10^{-10} \exp(-48300/T) cm^3 molecule^{-1} s^{-1}$, M = Ar	±0.3
18,19	$H + HO \rightarrow H_2 + O$		see reverse reaction	
18,19M	$H + HO + M \rightarrow H_2O + M$ (f)			
22,M	$H_2O + M \rightarrow H + HO + M$ (r)			
	*Baulch, et al (1972) review	1000-3000	$k_f = 6.1 \times 10^{-26} T^{-2}$ $cm^6 molecule^{-2} s^{-1}$, M = N_2	±0.3
		2000-6000	$k_r = 5.8 \times 10^{-9} \exp(-52900/T)$ $cm^3 molecule^{-1} s^{-1}$ M = N_2	±0.2
	Zellner, Erler, Field (1977)	230-300	$k_f = 4.3 \times 10^{-25} T^{-2.6}$ M = He Rel eff: He(1.0), Ar(1.5), N_2(3.2)	
18,20	$H + HO_2 \rightarrow HO + HO$ (1f)			
19,19	$HO + HO \rightarrow H + HO_2$ (1r)			
18,20	$H + HO_2 \rightarrow H_2 + O_2$ (2)			
18,20	$H + HO_2 \rightarrow H_2O + O$ (3)			
	Baulch, et al (1972) review	290-800	$k_{1f} = 4.2 \times 10^{-10} \exp(-950/T)$	±0.3 (a)
			$k_{1r} = k_{1f}/K_{eq} = 2.0 \times 10^{-11} \exp(-20200/T)$	±0.3
		290-800	$k_2 = 4.2 \times 10^{-11} \exp(-750/T)$	±0.4
			$k_{2r} = k_{2f}/K_{eq} = 9.1 \times 10^{-11} \exp(-29100/T)$	±0.4
			k_3 = no recommendation	
	Lloyd (1974) review	300-1000	k_{1f} and k_2 = same as Baulch, et al	>±0.3 (a)
			$k_3 = 8.3 \times 10^{-11} \exp(-500/T)$	>±0.5 (b)
	Moortgat, Allen (1973)	297	$k_{1f} = 8.3 \times 10^{-12}$	? (c)
			$k_2 = 1 \times 10^{-11}$	? (c)
			$k_3 = 6.7 \times 10^{-12}$	? (c)
			(a) Reaction 1 and rate ratios control values for reactions 2 and 3. (b) Temperature coefficient estimated. (c) Secondary reaction in $H + O_2 + M$ systems, fit of concentration vs. time plots.	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
18,22	$H + H_2O \rightarrow H_2 + HO$			
	Baulch, et al (1972) review	300-2500	$1.5 \times 10^{-10} \exp(-10250/T)$	±0.06 at 300K increasing to ±0.2 at high temp.
18,23	$H + H_2O_2 \rightarrow H_2 + HO_2$ (a) $\rightarrow HO + H_2O$ (b)			
	*Klemm, Payne, Stief (1975)	283-353	$k_a + k_b = 5.2 \pm 2.0 \times 10^{-12} \exp(-1400 \pm 140/T)$	
	Gorse, Volman (1974)	300	$k_a = 3.1 \pm 0.8 \times 10^{-15}$ $k_b = 5.7 \pm 1.4 \times 10^{-15}$	
	Hampson, et al (1973)	300-800	$k_a = 2.8 \times 10^{-12} \exp(-1900/T)$ k_b no recommendation (a) Accepts recommendations of Baulch, et al (1972).	(a) (a)
	Meagher, Heicklen (1975)	298	$k_b/k_a = 1.3$	
18,24	$H + HNO \rightarrow H_2 + NO$			
	Hampson, et al (1973) review	211-703	$> 5 \times 10^{-14}$	±0.3
		2000	7×10^{-12}	±0.3
	Baulch, et al (1973) review	300	$10^{-13} < k < 10^{-12}$	
		2000	8×10^{-12}	±0.2
18,25	$H + HNO_2 \rightarrow$ products			
	Hampson, et al (1973) review		No data	
	Baulch, et al (1973) review		No recommendation	
18,26	$H + HNO_3 \rightarrow$ products			
	Hampson, et al (1973) review	300	$< 1 \times 10^{-13}$	
	Chapman, Wayne (1974)	300	$< 2 \times 10^{-15}$	
	Baulch, et al (1973) review	300	$< 10^{-13}$	approximate upper limit
18,28M	$H + SO_2 + M \rightarrow HSO_3 + M$			
	Baulch, et al (1976) review	1660-2120	1.4×10^{-32}	±0.2
18,31	$H + HS \rightarrow H_2 + S$ (f)			
21,26a	$H_2 + S \rightarrow H + HS$ (r)			
	Baulch, et al (1976) review	298	$k_f = 2.5 \times 10^{-11}$	±0.2
			$k_r = 2.2 \times 10^{-25}$ (a) $k_r = k_f/K_{eq}$	±0.2 (a)
	Cupitt, Glass (1974)	295	$k_f = 2.5 \pm 0.8 \times 10^{-11}$	
18,32	$H + H_2S \rightarrow H_2 + HS$			
	Kurylo, Peterson, Braun (1971)	190-464	$1.29 \times 10^{-11} \exp(860/T)$ (a) Selected by Baulch, et al (1976) review	(a)
18,34c	$H + COS \rightarrow CO + HS$			
	Baulch, et al (1976) review	300	2.2×10^{-14}	±0.2
18,37	$H + OClO \rightarrow HO + ClO$			
	*Watson (1977) review	298	$5.7 \pm 1.2 \times 10^{-11}$	

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18,39	$H + HCl \rightarrow H_2 + Cl$			
	Ambidge, et al (1976a)	298-521	$7.8 \times 10^{-12} \exp(-1600 \pm 84/T)$	
	Spencer, Glass (1975)	295	4.3×10^{-14}	
18,42	$H + NOCl \rightarrow HCl + NO$			
	Wagner, et al (1976a)	255-461	$7.6 \times 10^{-11} \exp(-457 \pm 72/T)$	
18,44	$H + Cl_2 \rightarrow HCl + Cl$			
	*This survey	250-700	$1.46 \times 10^{-10} \exp(-593/T)$	±0.1 (a)
			(a) Based on data in Bemand, Clyne and Wagner, et al	
	Bemand, Clyne (1977)	300-730	$(1.41 \pm 0.24) \times 10^{-10} \exp(-575 \pm 65/T)$	
	Wagner, et al (1976)	252-458	$(1.44 \pm 0.28) \times 10^{-10} \exp(-600 \pm 70/T)$	
	Ambidge, et al (1976)	292-434	$(7.6 \pm 2.2) \times 10^{-11} \exp(-714 \pm 100/T)$	
18,45M	$H + CO + M \rightarrow HCO + M$			
	Baulch, et al (1976) review	298-773	$2.0 \times 10^{-33} \exp(-850/T)$, $M = H_2$	±0.12
18,46	$H + CO_2 \rightarrow HO + CO$		see reverse reaction	
18,48	$H + CH_2O \rightarrow H_2 + CHO$			
	Ridley, et al (1972)	297	5.4×10^{-14}	±0.04
	Westenberg, deHaas (1972b)	297-652	$2.2 \times 10^{-11} \exp(-1890/T)$	
18,53	$H + CH_3OOH \rightarrow CH_3O + H_2O$ (a)			
	$\rightarrow CH_3O_2 + H_2$ (b)			
	$\rightarrow CH_2OOH + H_2$ (c)			
	Slemr, Warneck (1977)	250-358	$k = (2.8 \pm 0.9) \times 10^{-13} \exp(-930 \pm 95/T)$ overall rate const	
			$k_a/k = 0.43 \pm 0.07$	
			$k_b/k = 0.52 \pm 0.07$	
			$k_c/k = 0.05$	
18,54	$H + CH_3ONO \rightarrow CH_3OH + NO$ (a)			
	$\rightarrow CH_2ONO + H_2$ (b)			
	$\rightarrow CH_3O + HNO$ (c)			
	Moortgat, et al (1977)	223-398	$k = (4.3 \pm 0.9) \times 10^{-13} \exp(-950 \pm 55/T)$ overall rate const	
			$k_a/k = 0.47 \pm 0.05$	
			$(k_b + k_c)/k = 0.53 \pm 0.05$	
18,64	$H + CH_3Cl \rightarrow HCl + CH_3$			
	Westenberg, deHaas (1975a)	500-800	$6.2 \times 10^{-11} \exp(-4650/T)$	
19,M	$HO + M \rightarrow H + O + M$			
	Baulch, et al (1972) review		no recommendation (E/R > 50000 K)	
19,19	$HO + HO \rightarrow H + HO_2$		see reverse reaction	
19,19	$HO + HO \rightarrow H_2 + O_2$			
	Baulch, et al (1972) review		no recommendation	
19,19	$HO + HO \rightarrow H_2O + O$ (f)			
1,22	$O + H_2O \rightarrow HO + HO$ (r)			
	*Baulch, et al (1972) review	300-2000	$k_f = 1.0 \times 10^{-11} \exp(-550/T)$	±0.2
		300-2000	$k_r = 1.1 \times 10^{-10} \exp(-9240/T)$	±0.2
	Rawlins, Gardiner (1974)	1500-2000	$k_f = 9.1 \times 10^{-11} \exp(-3500/T)$	
	Westenberg, deHaas (1973a)	300	$k_r = 2.3 \times 10^{-12}$	±0.06

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
	McKenzie, et al (1973)	298	$k_f = 2.1 \pm 0.5 \times 10^{-12}$	
	Clyne, Down (1974)	300	$k_f = 1.4 \pm 0.2 \times 10^{-12}$	
		300	$k_f = 1.7 \pm 0.6 \times 10^{-12}$	(a)
	Trainor, von Rosenberg (1974)	300	$k_f = 2.1 \pm 0.2 \times 10^{-12}$	
	Wilson (1972) review	300	$k_f = 2.57 \times 10^{-12}$ (a) Evaluation based on authors' work and other recent data	+0.1, -0.5
19,19M 23,M	$H\emptyset + H\emptyset + N \rightarrow H_2\emptyset_2 + M$ (f) $H_2\emptyset_2 + M \rightarrow H\emptyset + H\emptyset + M$ (r)		$-d[\emptyset H]/dt = 2k[\emptyset H]^2[M]$	
	†*NASA (1977) eval	200-300	$k_f = 1.25 \times 10^{-32} \exp(900/T)$ (a) Accepts room temp value of Trainor, von Rosenberg. E/R value chosen same as for comb. of ØH with NØ	(a)
	Trainor, von Rosenberg (1974)	300	$k_f = 2.5 \pm 0.3 \times 10^{-31}$ M = N_2	
	Baulch, et al (1972) review	700-1500	$k_f = 2.5 \times 10^{-33} \exp(+2550/T) cm^6 molecule^{-2} s^{-1}$ M = N_2 $k_r = 2.0 \times 10^{-7} \exp(-22900/T) cm^3 molecule^{-1} s^{-1}$, M = N_2; $k_f = k_r K_{eq}$	±0.1 700<T<950K ±0.3 at 1500K
19,20	$H\emptyset + H\emptyset_2 \rightarrow H_2\emptyset + \emptyset_2$			
	†*NASA (1977) eval	200-300	3×10^{-11}	0.5 at 230K
	Burrows, Harris, Thrush (1977)	293	5.1×10^{-11} (a) Based on $k(H\emptyset + H_2\emptyset_2) = 7.9 \times 10^{-13}$	(a)
	Lloyd (1974) review	300-1000	$8.3 \times 10^{-11} \exp(-500/T)$	±0.3
	Hochanadel, et al (1972)	300	2×10^{-10}	
	DeMore, Tschuikow-Roux (1974)	300	1.1×10^{-10} (a) Adjusted value - based on reported ratio and values of $k(\emptyset_3 + H\emptyset)$ and $k(H\emptyset_2 + H\emptyset_2)$ in this survey.	±0.5 (a)
19,21	$H\emptyset + H_2 \rightarrow H_2\emptyset + H$			
	*Baulch, et al (1972) review	300-2500	$3.6 \times 10^{-11} \exp(-2590/T)$ $cm^3 molecule^{-1} s^{-1}$	±0.08 at 300K ±0.2 at high temp.
	Wilson (1972) review	300-2000	$3.8 \times 10^{-11} \exp(-2600/T)$	±0.3
	Stuhl, Niki (1972)	298	7.1×10^{-15}	±0.06
	Westenberg (1973a)	298	7.6×10^{-15}	±0.04
		352	1.8×10^{-14}	
		403	3.2×10^{-14}	
		518	1.4×10^{-13}	
		628	3.6×10^{-13}	
		745	6.6×10^{-13}	
	Smith, Zellner (1974a)	210-460	$1.8 \times 10^{-11} \exp(-2330/T)$	
	Gardiner, et al (1974)	1350-1600	$8.7 \times 10^{-11} \exp(-3250/T)$	
	Greiner (1969)	300-500	$6.8 \times 10^{-12} \exp(-2020/T)$	±0.15
	Atkinson, Hansen, Pitts (1975)	297-434	$5.9 \times 10^{-12} \exp(-2008 \pm 150/T)$	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
	Overend, et al (1975)	295	$(5.80 \pm 0.26) \times 10^{-15}$	
	Trainor, von Rosenberg (1975)	300	5.3×10^{-15}	
	Vandooren, et al (1975)	600-1300	$1.2 \times 10^{-11} \exp(-2200/T)$	
19,21	$H\dot{O} + D_2 \rightarrow HD\dot{O} + D$			
	Smith, Zellner (1974a)	210-460	$1.25 \times 10^{-11} \exp(-2590/T)$	
19,22	$H\dot{O} + H_2\dot{O} \rightarrow H_2\dot{O}_2 + H$			
	Baulch, et al (1972) review		no recommendation	
19,23	$H\dot{O} + H_2\dot{O}_2 \rightarrow H_2\dot{O} + H\dot{O}_2$			
	†*NASA (1977) eval	200-300	$1 \times 10^{-11} \exp(-750/T)$	±0.3 at 230K (a)
	Hack, et al (1975)	298-670	$8.0 \times 10^{-12} \exp(-670/T)$	
	Greiner (1968)	300-458	$4.1 \times 10^{-13} T^{1/2} \exp(-600/T)$	
	Hampson (1973) quoting Baulch, et al (1972) review	300-800	$1.7 \times 10^{-11} \exp(-910/T)$	±0.?
	Gorse, Volman (1972)	300	$k/k(H\dot{O} + C\dot{O}) = 8.13$	
	Meagher, Heicklen (1974)	298	$k/k(H\dot{O} + C\dot{O}) = 4.1 \pm 0.6$	
			(a) Based on results of Hack, et al (1975) and Greiner (1968)	
19,24	$H\dot{O} + HN\dot{O} \rightarrow H_2\dot{O} + N\dot{O}$			
	Hampson, et al (1973) review	1600-2100	7×10^{-11}	±0.7
	Baulch, et al (1973) reviw	2000	6×10^{-11}	±0.2
19,25	$H\dot{O} + HN\dot{O}_2 \rightarrow H_2\dot{O} + N\dot{O}_2$			
	Cox, Derwent, Holt (1976)	296	$(6.6 \pm 0.3) \times 10^{-12}$ ref. rxn is $H\dot{O} + H_2 \rightarrow H_2\dot{O} + H$ with $k_{ref} = 7 \times 10^{-15}$	
	Cox (1974a)	294	$k/k(H\dot{O} + C\dot{O}) = 15 \pm 1$ at 1 atm air	
19,26	$H\dot{O} + HN\dot{O}_3 \rightarrow H_2\dot{O} + N\dot{O}_3$			
	†*Smith, Zellner (1975)	240-406	$8 \pm 2 \times 10^{-14}$	±0.1 at 230K (a)
	Margitan, et al (1975)	270-470	$8.9 \pm 1.3 \times 10^{-14}$	
	Hampson, et al (1973) review	300-650	$6 \times 10^{-13} \exp(-400/T)$	±0.5
	Johnston (1974) review	300-700	$(1.5 \text{ to } 2.0) \times 10^{-13}$	±0.?
	Baulch, et al (1973) review	300	1.3×10^{-13}	±0.3
			(a) Value recommended by authors for $T \leq 298K$.	
19,28M	$H\dot{O} + S\dot{O}_2 + M \rightarrow HS\dot{O}_3 + M$			
	Davis (1976)	300	$10^{13} \times k$ / P(He)/torr 0.87 ± 0.06 / 50 1.6 ± 0.1 / 150 2.7 ± 0.2 / 500 $10^{13} \times k$ / P(Ar)/torr 1.37 ± 0.06 / 50 2.50 ± 0.3 / 150 3.71 ± 0.3 / 500 $10^{13} \times k$ / $P(N_2)$/torr 0.08 ± 0.08 / 5 1.43 ± 0.14 / 10	(a)

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
			2.44 ± 0.3 20	
			~9 (b) 760	
			(b) Extrapolated value.	
	Harris, Wayne (1975)	300	$4.5 \pm 1.5 \times 10^{-31}$ $cm^6 molecule^{-2} s^{-1}$, M = Ar	
			$7.2 \pm 2.6 \times 10^{-31}$, M = N_2	
	Cox (1974a)	294	k/k(HO + CO) = 4 ± 0.5	(c)
			(c) 2nd order rate constant, [M] = 1 atm. N_2 + O_2 see entry for k(HO + CO)	
	Gordon, Mulac (1975)	435	1.8×10^{-12} $cm^3 molecule^{-1} s^{-1}$ (2d order rate constant at 1 atm. H_2O vapor)	
	Castleman, Tang (1977)	297	$1.6 \times 10^{-31} cm^6 molecule^{-2} s^{-1}$, M = N_2	
			k/k(HO + CO) = 4.3	(d)
			(d) Measured ratio of 2d order rate constants at 1 atm N_2. Values for k given in paper assumed $k_{ref} = 1.5 \times 10^{-13}$ over entire pressure range. See entry for k(OH + CO)	
	Atkinson, Perry, Pitts (1976)	298	10^{13} x k / P(Ar)/torr	(e)
			1.35 / 25	
			2.16 / 50	
			3.10 / 100	
			4.38 / 202	
			5.87 / 402	
			6.55 / 648	
			(e) Effective 2nd order rate constant in $cm^3 molecule^{-1} s^{-1}$	
19,32	HO + H_2S → H_2O + HS			
	Baulch, et al (1976) review	300-500	$1.05 \times 10^{-11} exp(-200/T)$	±0.15
	Perry, Atkinson, Pitts (1976a)	297-427	$(5.2 \pm 0.5) \times 10^{-12}$	
	Stuhl (1974)	298	$3.1 \pm 0.5 \times 10^{-12}$	
19,35	HO + Cl → O + HCl		see reverse reaction	
19,39	HO + HCl → H_2O + Cl			
	†*Watson (1977) review	220-300	$3.0 \times 10^{-12} exp(-425/T)$	±0.1 at 230K
	Smith, Zellner (1974a)	210-460	$4.1 \times 10^{-12} exp(-530/T)$	
	Zahniser, et al (1974)	224-460	$2.0 \pm 0.1 \times 10^{-12} exp(-312 \pm 10/T)$	
	Takacs, Glass (1973)	295	$6.4 \pm 1.5 \times 10^{-13}$	±0.1
	Davis (1974)	300	$6.5 \pm 0.4 \times 10^{-13}$	
19,39	HO + DCl → HDO + Cl			
	Smith, Zellner (1974a)	210-460	$4.7 \times 10^{-12} exp(-780/T)$	
19,39Br	HO + HBr → H_2O + Br			
	†*Takacs, Glass (1973)	300	5.1×10^{-12}	±0.36 at 230K
19,43a	HO + NO_3Cl → products			
	†*Zahniser, et al (1977)	246-387	$(1.19 \pm 0.10) \times 10^{-12} exp(-333 \pm 22/T)$	±0.36 at 230K
	Ravishankara, et al (1977)	245	3.7×10^{-13}	
19,45	HO + CO → CO_2 + H (f)			
18,46	H + CO_2 → HO + CO (r)			
	†NASA (1977) eval	200-400	$k_f = 1.4 \times 10^{-13}$ low pressure value	±0.1

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant k/cm^{3}molecule^{-1}s^{-1}	Notes and Reliability of log k
	*Baulch, et al (1976) review	250-2500	$\log k_f = -12.95 + 3.94 \times 10^{-4} \times T$ same as given in Baulch, Drysdale (1974)	±0.1
		1000-3000	$k_r = k_f/K_{eq} = 2.5 \times 10^{-10} \exp(-13300/T)$ recommendation based on low pressure studies	±0.1
	*This survey	300	$k_f = 3.0 \times 10^{-13}$ 1 atmosphere air	±0.1 (a)
			(a) Tentative rec. Recent experiments at room temperature have shown an apparent increase in k in the presence of SF_6, H_2, N_2/O_2 but not He or Ar. Biermann, et al (1978) have identified a combined effect of inert gas and O_2. Trace impurities of O_2 have a significant effect and 1 torr is sufficient to produce the limiting rate constant in the presence of 1 atm of N_2.	
			Experiments bearing on the "pressure effect"	
	Butler, et al (1977)	298	k_f/k_{ref} / P/torr / Mole fractions $N_2/O_2/CO$ 0.094 / 100 / 0.49/0.33/0.15 0.10 / 200 / 0.50/0.34/0.15 0.17 / 300 / 0.73/0.17/0.08 0.15 / 400 / 0.50/0.34/0.15 0.16 / 500 / 0.73/0.17/0.07 0.18 / 600 / 0.74/0.17/0.08 Ref. rxn is HO + isobutane → products, with 6-28% correction for side rxn. Ratios calculated from reported data using authors' value for $k_{ref} = 1.59 \times 10^{-12}$ which was determined in the 100 torr expt. relative to $k(HO + CO) = 1.5 \times 10^{-13}$	
	Chan, et al (1977)	298	k_f/k_{ref} / P/torr 0.059 / 100 in "synthetic air" 0.127 / 700 Ref. rxn is HO + isobutane → products	
	Sie, Simonaitis, Heicklen (1976a)	217-298	k_f/k_{ref} / P/torr 0.2exp(1700/T) / high pressure limit in H_2	
		298	14 / 20 (H_2) 21 / 83 (H_2) 42 / 296 (H_2) 49 / 702 (H_2) 17 / 605 (He) + 2O (H_2) 33 / 550 (SF_6) + 2O (H_2) 49 / 605 (SF_6) + 2O (H_2)	
			Ref. rxn is HO + H_2 → H_2O + H	
	Cox, Derwent, Holt (1976)	296	k_f/k_{ref} / P/torr 38.6 / 700 N_2/O_2 = 2 Ref. rxn. is HO + H_2 → H_2O + H	
	Atkinson, Perry, Pitts (1976)	299	$(1.54 \pm 0.16) \times 10^{-13}$ P = 25-654 torr Ar	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
	Perry, Atkinson, Pitts (1977a)	299	10^{13} x k / $P(SF_6)$/torr 1.53 / 25 1.93 / 76 2.40 / 208 3.09 / 403 3.43 / 603	
	Overend, Paraskevopoulos (1977)	296	$(2.03 \pm 0.08) \times 10^{-13}$ at 50 torr He $(3.24 \pm 0.20) \times 10^{-13}$ at 200, 350 torr SF_6	
	Gordon, Mulac (1975)	298	1.50×10^{-13} at 710 torr Ar, 10 torr H_2O	
			Experiments either at low pressure or for which pressure effects were not studied.	
	Trainor, von Rosenberg (1975)	300	1.25×10^{-13}	
	Vandooren, et al (1975)	400-800	1.33×10^{-13}	
		1000-1800	$3.85 \times 10^{-12} \exp(-2850/T)$	
	Biordi, et al (1975)	1350-1750	7.8×10^{-13}	
	Steinert, Zellner (1975)	300-900	$\log k = -12.93 + 4.0 \times 10^{-4} \times T$	
	Wilson (1972) review	300-2000	$5.1 \times 10^{-13} \exp(-300/T)$	±0.3
	Stuhl, Niki (1972)	300	1.35×10^{-13}	±0.06
	Westenberg, deHaas (1973a)	298	1.33×10^{-13}	±0.04
		396	1.38×10^{-13}	
		523	1.44×10^{-13}	
		707	1.69×10^{-13}	
		915	2.17×10^{-13}	
	Davis, Fischer, Schiff (1974)	220-373	$2.15 \pm 0.19 \times 10^{-13} \exp(-80 \pm 40/T)$	±0.04
	Greiner (1969)	300-500	$2.1 \times 10^{-13} \exp(-115/T)$	±0.1
	Smith, Zellner (1973)	300	1.45×10^{-13}	(b)
			(b) Data reported 210 <T< 460 K. Slight positive temperature dependence, possibly curved.	
	Peeters, Mahnen (1973)	1600-1900	4.7×10^{-13}	
	Gardiner, et al (1973)	1500-2000	$6.7 \times 10^{-12} \exp(-4000/T)$	
	Howard, Evenson (1974)	296	$1.56 \pm 0.2 \times 10^{-13}$	
19,48	$HO + CH_2O \rightarrow H_2O + CHO$			
	†*NASA (1977) eval	200-300	$3 \times 10^{-11} \exp(-250/T)$	±0.4 at 230K (a)
	*Morris, Niki (1971)	300	1.4×10^{-11}	±0.1
	Wilson (1972) review	300-1600	8×10^{-11}	±1
	Peeters, Mahnen (1973)	1400-1800	3.8×10^{-11}	
			(a) "A factor" chosen; E_{act} fitted to room temp value of Morris, Niki	
19,52	$HO + CH_3OH \rightarrow$ products			
	Campbell, et al (1976)	292	9.5×10^{-13}	
19,54	$HO + CH_3NO_2 \rightarrow$ products			
	Campbell, Goodman (1975b)	292	9.2×10^{-13}	
19,54	$HO + CH_3ONO \rightarrow$ products			
	Campbell, Goodman (1975b)	292	1.3×10^{-12}	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
19,56	$H\dot{O} + CH_4 \rightarrow CH_3 + H_2O$			
	†*Davis, Fischer, Schiff (1974)	240-373	$2.36 \pm 0.21 \times 10^{-12} \exp(-1710 \pm 88/T)$	±0.04
	Margitan, et al (1974)	290-440	$3.83 \times 10^{-12} \exp(-1840 \pm 20/T)$	±0.06
	Wilson (1972) review	300-2000	$4.7 \times 10^{-11} \exp(-2500/T)$	±0.7
	Øverend, et al (1975)	300	$6.51 \pm 0.26 \times 10^{-15}$	
	Peeters, Mahnen (1973)	1100-1900	$5 \times 10^{-11} \exp(-3000/T)$	
	Greiner (1970)	300-500	$5.5 \times 10^{-12} \exp(-1900/T)$	±0.1
	Gordon, Mulac (1975)	381	2.6×10^{-14} (1 atm H_2O vapor)	
		416	5.5×10^{-14} (1 atm H_2O vapor)	
	Zellner, Steinert (1976)	300-900	$5.76 \times 10^{-21} T^{3.08} \exp(-1010/T)$	
	Howard, Evenson (1976)	296	$(9.5 \pm 1.4) \times 10^{-15}$	
	Cox, Derwent, Holt (1976)	296	$(7.3 \pm 0.9) \times 10^{-15}$ ref rxn is $H\dot{O} + H_2 \rightarrow H_2O + H$ with $k_{ref} = 7 \times 10^{-15}$	
19,56a	$H\dot{O} + C_2H_2 \rightarrow$ products			
	Smith, Zellner (1973)	210-460	$2.0 \times 10^{-12} \exp(-250/T)$	
	Pastrana, Carr (1974)	300	$2.0 \pm 0.6 \times 10^{-13}$	
	Davis, et al (1975)	300	$1.65 \pm 0.15 \times 10^{-13}$	
19,57	$H\dot{O} + C_2H_4 \rightarrow$ products			
	Atkinson, Perry, Pitts (1977)	299-425	$2.2 \times 10^{-12} \exp(385 \pm 150/T)$	(a)
			(a) High pressure values (225-660 torr Ar) Values also given for 25 and 75 torr pressure dependent values given over range 1 to 7 torr He	
	Howard (1976)	296	$1.0 \pm 0.2 \times 10^{-11}$	(b)
	Øverend, Paraskevopoulos (1977)	296	(b) Authors' suggested limiting high pressure value based on expts at 400 torr SF_6 and CF_4 and analysis of dependence of k on $[H_2O]$ at low values of $[H_2O]$	
	Stuhl (1973c)	298	3×10^{-12}	±0.12
	Smith, Zellner (1973)	210-460	$7.5 \times 10^{-12} \exp(-110/T)$	
	Davis, et al (1975)	300	$10^{12} \times k$ / P(He)/torr: 2.24 / 3 2.78 / 5 3.63 / 10 4.06 / 20 4.72 / 100 5.33 / 300	
		300	3.64×10^{-12} at 3 torr N_2	
	Morris, et al (1971)	300	1.8×10^{-12}	
	Bradley, et al (1973)	300	$1.7 \pm 0.5 \times 10^{-12}$	
	Greiner (1970a)	300-500	$1.26 \times 10^{-12} \exp(454/T)$ at 100 torr He	
	Gordon, Mulac (1975)	381	6.2×10^{-12} (1 atm H_2O vapor)	
		416	7.3×10^{-12} (1 atm H_2O vapor)	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
19,58	$H\emptyset + C_2H_6 \rightarrow$ products			
	Øverend, et al (1975)	300	$2.64 \pm 0.17 \times 10^{-13}$	
	Greiner (1970)	300-500	$1.86 \times 10^{-11} \exp(-1230/T)$	
	Howard, Evenson (1976)	296	$(2.9 \pm 0.6) \times 10^{-13}$	
19,59	$H\emptyset + C_3H_6 \rightarrow$ products			
	Atkinson, Pitts (1975b)	297-425	$4.1 \times 10^{-12} \exp(540 \pm 150/T)$	
	Stuhl (1973c)	298	1.45×10^{-11}	±0.06
	Morris, et al (1971)	300	1.7×10^{-11}	
	Bradley, et al (1973)	300	$5.0 \pm 1.7 \times 10^{-12}$	
	Gorse, Volman (1974)	300	$k/k(C\emptyset + H\emptyset) = 89.3$ (low pressure) $k = 1.2 \times 10^{-11}$ (a) $k(C\emptyset + H\emptyset) = 1.4 \times 10^{-13}$, this survey	(a)
	Davis (1976)	300	$1.53 \pm 0.06 \times 10^{-11}$	
	Gordon, Mulac (1975)	381	1.4×10^{-11} (1 atm $H_2\emptyset$ vapor)	
		416	2.0×10^{-11} (1 atm $H_2\emptyset$ vapor)	
19,60	$H\emptyset + n\text{-}C_4H_{10} \rightarrow$ products			
	Stuhl (1973b)	300	2.35×10^{-12}	±0.06
	Perry, Atkinson, Pitts (1976b)	297-420	$1.76 \times 10^{-11} \exp(-560/T)$	
	Greiner (1970)	300-500	$1.41 \times 10^{-11} \exp(-524/T)$	
	Gorse, Volman (1974)	300	$k/k(C\emptyset + H\emptyset) = 19.4$ (low pressure) $k = 2.7 \times 10^{-12}$ (a) $k(C\emptyset + H\emptyset) = 1.4 \times 10^{-13}$, this survey	(a)
19,60	$H\emptyset +$ isobutane $\rightarrow$ products			
	Greiner (1970)	300-500	$8.7 \times 10^{-12} \exp(-387/T)$	
	Gorse, Volman (1974)	300	$k/k(H\emptyset + C\emptyset) = 23.5$ (low pressure) $k = 3.3 \times 10^{-12}$ (a) $k(C\emptyset + \emptyset H) = 1.4 \times 10^{-13}$, this survey	(a)
	Butler, et al (1977)	300	1.6×10^{-12} (b) Determined in expt. at 100 torr relative to $k(H\emptyset + C\emptyset) = 1.5 \times 10^{-13}$	(b)
19,60	$H\emptyset +$ alkane $\rightarrow H_2\emptyset +$ alkyl radical			
	Greiner (1970)	300-500	$k = [1.0 \exp(-820/T) N_p + 2.3 \exp(-430/T) N_s + 2.1 \exp(+95/T) N_t] \times 10^{-12}$ Where N_p, N_s, and N_t are the number of primary secondary, and tertiary hydrogen atoms respectively. Do not use formula for CH_4 and C_2H_6.	
19,60a	$H\emptyset + C_6H_6 \rightarrow$ products			
	Perry, Atkinson, Pitts (1977)	298	$(1.20 \pm 0.15) \times 10^{-12}$ total rxn; P = 100 torr Ar	
		380-470	$k_1 = 4 \times 10^{-11} \exp(-2000/T)$	(a)
		298	$k_1/k = 0.05$	(b)
			(a) k_1 refers to abstraction rxn (b) Fraction of rxn proceeding by abstraction; expression for k_1 extrapolated to 298K	
	Hansen, Atkinson, Pitts (1975)	298	$(1.24 \pm 0.12) \times 10^{-12}$ total rxn; P = 50-600 torr Ar	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
	Davis, Bollinger, Fischer (1975)	298	0.85×10^{-12} P = 3 torr He	total rxn
			1.36×10^{-12} P = 20 torr He	total rxn
			1.59×10^{-12} P = 100 torr He	total rxn
19,60a	$H\dot{O} + C_6H_5CH_3 \rightarrow$ products			
	Perry, Atkinson, Pitts (1977)	298	$(6.40 \pm 0.64) \times 10^{-12}$	total rxn; P = 200 torr Ar
		380-470	$k_1 = 5 \times 10^{-12} \exp(-450/T)$	(a)
		298	$k_1/k = 0.16$	(b)
			(a) k_1 refers to H atom abstraction	
			(b) Fraction of rxn proceeding by abstraction: expression for k_1 extrapolated to 298K	
	Hansen, Atkinson, Pitts (1975)	298	$(5.78 \pm 0.58) \times 10^{-12}$	total rxn: P = 100-600 torr Ar
	Davis, Bollinger, Fischer (1975)	298	3.60×10^{-12} P = 3 torr He	total rxn
			5.00×10^{-12} P = 20 torr He	total rxn
			6.11×10^{-12} P = 100 torr He	total rxn
19,61	$H\dot{O} + CF_2Cl_2 \rightarrow$ products			
	†*NASA (1977) eval	200-300	$k < 1 \times 10^{-12} \exp(-3560/T)$	(a,b)
	Atkinson, Hansen, Pitts (1975)	297-424	$k < 1 \times 10^{-15}$	(a)
	Howard, Evenson (1976a)	296	$k < 4 \times 10^{-16}$	(a)
	Chang, Kaufman (1977)	480	$k < 6 \times 10^{-16}$	(a)
			(a) upper limit only	
			(b) Expression based on upper limit at 480K reported by Chang and Kaufman. "A factor" chosen; E/R value derived	
19,62	$H\dot{O} + CFCl_3 \rightarrow$ products			
	†*NASA (1977) eval	200-300	$k < 1 \times 10^{-12} \exp(-3650/T)$	(a,b)
	Atkinson, Hansen, Pitts (1975)	297-424	$k < 1 \times 10^{-15}$	(a)
	Howard, Evenson (1976a)	296	$k < 5 \times 10^{-16}$	(a)
	Chang, Kaufman (1977)	480	$k < 5 \times 10^{-16}$	(a)
			(a) upper limit only	
			(b) Expression based on upper limit at 480K reported by Chang and Kaufman. "A factor" chosen; E/R value derived	
19,63	$H\dot{O} + CCl_4 \rightarrow$ products			
	Howard, Evenson (1976a)	296	$k < 4 \times 10^{-15}$	upper limit only
19,64	$H\dot{O} + CH_3Cl \rightarrow H_2\dot{O} + CH_2Cl$			
	†*NASA (1977) eval	200-300	$2.2 \times 10^{-12} \exp(-1142/T)$	±0.2 at 230K
	Davis, et al (1976)	250-350	$(1.84 \pm 0.18) \times 10^{-12} \exp(-1098 \pm 35/T)$	
	Perry, Atkinson, Pitts (1976)	298-423	$4.1 \times 10^{-12} \exp(-1359 \pm 150/T)$	
	Howard, Evenson (1976a)	296	$(3.6 \pm 0.8) \times 10^{-14}$	
19,64	$H\dot{O} + CH_2Cl_2 \rightarrow H_2\dot{O} + CHCl_2$			
	†*NASA (1977) eval	200-300	$5.2 \times 10^{-12} \exp(-1094/T)$	±0.2 at 230K
	Davis, et al (1976)	245-375	$(4.27 \pm 0.63) \times 10^{-12} \exp(-1094 \pm 81/T)$	
	Perry, Atkinson, Pitts (1976)	298	$(1.45 \pm 0.20) \times 10^{-13}$	
	Howard, Evenson (1976)	296	$(1.55 \pm 0.14) \times 10^{-13}$	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
19,64	$H\dot{O} + CHCl_3 \rightarrow H_2O + CCl_3$			
	†*Davis, et al (1976)	245-375	$(4.69 \pm 0.71) \times 10^{-12} \exp(-1134 \pm 108/T)$	±0.2 at 230K
	Howard, Evenson (1976a)	296	$1.01 \pm 0.15 \times 10^{-13}$	
19,65	$H\dot{O} + CHFCl_2 \rightarrow H_2O + CFCl_2$			
	†*NASA (1977) eval	200-300	$1.3 \times 10^{-12} \exp(-1127/T)$	±0.2 at 230K
	Perry, Atkinson, Pitts (1976)	298-422	$1.75 \times 10^{-12} \exp(-1253 \pm 150/T)$	
	Chang, Kaufman (1977)	241-396	$(1.16 \pm 0.17) \times 10^{-12} \exp(-1073 \pm 40/T)$	
	Watson, et al (1977)	245-375	$(1.87 \pm 0.2) \times 10^{-12} \exp(-1245 \pm 26/T)$	
	Howard, Evenson (1976a)	296	2.6×10^{-14}	
19,65	$H\dot{O} + CHF_2Cl \rightarrow H_2O + CF_2Cl$			
	†*NASA (1977) eval	200-300	$1.2 \times 10^{-12} \exp(-1660/T)$	±0.08 at 230K
	Atkinson, Hansen, Pitts (1975)	297-434	$1.21 \times 10^{-12} \exp(-1636 \pm 150/T)$	
	Chang, Kaufman (1977)	253-427	$(1.20 \pm 0.16) \times 10^{-12} \exp(-1657 \pm 39/T)$	
	Watson, et al (1977)	250-350	$(9.25 \pm 1.0) \times 10^{-13} \exp(-1575 \pm 71/T)$	
	Howard, Evenson (1976a)	296	3.4×10^{-15}	
19,65	$H\dot{O} + CH_2FCl \rightarrow H_2O + CHFCl$			
	†*Watson, et al (1977)	245-375	$(2.84 \pm 0.3) \times 10^{-12} \exp(-1259 \pm 50/T)$	±0.2
	Howard, Evenson (1976a)	296	$3.7 \pm 0.6 \times 10^{-14}$	
19,65	$H\dot{O} + CH_3F \rightarrow$ products			
	Howard, Evenson (1976a)	296	$16 \pm 2 \times 10^{-15}$	
19,65	$H\dot{O} + CH_2F_2 \rightarrow$ products			
	Howard, Evenson (1976a)	296	$7.8 \pm 1.2 \times 10^{-15}$	
19,65	$H\dot{O} + CHF_3 \rightarrow$ products			
	Howard, Evenson (1976a)	296	2×10^{-16}	
19,65	$H\dot{O} + CF_4 \rightarrow$ products			
	Howard, Evenson (1976a)	296	$k < 4 \times 10^{-16}$	upper limit only
19,65	$H\dot{O} + CF_3Cl \rightarrow$ products			
	Howard, Evenson (1976a)	296	$k < 7 \times 10^{-16}$	upper limit only
19,65	$H\dot{O} + CH_3Br \rightarrow H_2O + CH_2Br$			
	†*Davis, et al (1976)	245-350	$(7.93 \pm 0.79) \times 10^{-13} \exp(-889 \pm 98/T)$	±0.2 at 230K
	Howard, Evenson (1976a)	296	$35 \pm 8 \times 10^{-13}$	
19,65	$H\dot{O} + CH_3CCl_3 \rightarrow$ products			
	†*NASA (1977) eval	200-300	$3.5 \times 10^{-12} \exp(-1562/T)$	±0.36 at 230K
	Watson, et al (1977)	260-375	$(3.72 \pm 0.4) \times 10^{-12} \exp(-1627 \pm 50/T)$	
	Chang, Kaufman (1977)	275-405	$(1.95 \pm 0.24) \times 10^{-12} \exp(-1333 \pm 37/T)$	
	Howard, Evenson (1976b)	296	$15 \pm 3 \times 10^{-15}$	
19,65	$H\dot{O} + C_2HCl_3 \rightarrow$ products			
	†*NASA (1977) eval	200-300	2.3×10^{-12}	±0.3€
	Chang, Kaufman (1977)	234-420	$(5.32 \pm 0.71) \times 10^{-13} \exp(+445 \pm 41/T)$	
	Davis (1977)	300	$2.35 \pm 0.25) \times 10^{-12}$	preliminary
	Howard (1976)	296	$2.0 \pm 0.4 \times 10^{-12}$	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
19,65	$H\dot{O} + C_2Cl_4 \rightarrow$ products			
	†*Chang, Kaufman (1977)	297-420	$(9.44 \pm 1.34) \times 10^{-12} \exp(-1199 \pm 55/T)$	±0.36 at 230K
	Davis (1977)	260-375	$(1.06 \pm 0.5) \times 10^{-11} \exp(-1300 \pm 150/T)$	preliminary
	Howard (1976)	296	$1.70 \times 0.34 \times 10^{-13}$	
19,65	$H\dot{O} + CH_3CF_2Cl \rightarrow$ products			
	Watson, et al (1977)	273-375	$(1.15 \pm 0.15) \times 10^{-12} \exp(-1748 \pm 30/T)$	
	Howard, Evenson (1976b)	296	$2.8 \pm 0.4 \times 10^{-15}$	
19,65	$H\dot{O} + CF_2ClCFCl_2 \rightarrow$ products			
	Watson, et al (1977)	298	$k < 3 \times 10^{-16}$	upper limit only
20,M	$H\dot{O}_2 + M \rightarrow H + O_2 + M$		see reverse reaction	
20,M	$H\dot{O}_2 + M \rightarrow H\dot{O} + \dot{O} + M$		see reverse reaction	
20,20	$H\dot{O}_2 + H\dot{O}_2 \rightarrow H_2O_2 + O_2$		$-d[H\dot{O}_2]/dt = 2k[H\dot{O}_2]^2$	
	†*Hamilton, Lii (1977)	298	2.5×10^{-12} (a) Supersedes result reported in Hamilton (1975)	±0.3 (a)
	Baulch, et al (1972) review	300	3.3×10^{-12}	
	Lloyd (1974) review	300-1000	$1.7 \times 10^{-11} \exp(-500/T)$ Temperature coefficient	±0.3 at 300K larger at higher T
20,21	$H\dot{O}_2 + H_2 \rightarrow H_2O_2 + H$			
	Baulch, et al (1972) review	300-800	$1.2 \times 10^{-12} \exp(-9400/T)$	±0.3
	Lloyd (1974) review	300-1000	same recommendation. $k_f = k_r K_{eq}$	
20,22	$H\dot{O}_2 + H_2\dot{O} \rightarrow H_2O_2 + H\dot{O}$			
	Baulch, et al (1972) review	300-800	$4.7 \times 10^{-11} \exp(-16,500/T)$	±0.2
	Lloyd (1974) review	300-1000	same recommendation $k_f = k_r K_{eq}$	
20,28	$H\dot{O}_2 + S\dot{O}_2 \rightarrow S\dot{O}_3 + H\dot{O}$			
	*Payne, Stief, Davis (1973)	300	9×10^{-16} cm^{3}molecule^{-1}s^{-1} (a) Relative rate measurement. Value based on $k(H\dot{O}_2 + H\dot{O}_2)$ this survey.	±0.3 (a)
20,35	$H\dot{O}_2 + Cl \rightarrow HCl + O_2$			
	†*Leu, DeMore (1976)		3×10^{-11}	±0.6 at 230K
20,35Br	$H\dot{O}_2 + Br \rightarrow HBr + O_2$			
	†*NASA (1977) eval	200-300	5×10^{-12} (a) estimate - no data	±1.5 at 230K (a)
20,36	$H\dot{O}_2 + Cl\dot{O} \rightarrow H\dot{O}Cl + O_2$			
	†*NASA (1977) eval	200-300	2×10^{-13} (a) No data; value assumed to be intermediate between $k(H\dot{O}_2 + H\dot{O}_2)$ and $k(Cl\dot{O} + Cl\dot{O})$	±1 at 230K (a)
20,45	$H\dot{O}_2 + C\dot{O} \rightarrow C\dot{O}_2 + H\dot{O}$			
	*This survey	300	$<10^{-19}$	a
	Baulch, et al (1976) review	700-1000	$2.5 \times 10^{-10} \exp(-11900/T)$	±0.5

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
	Lloyd (1974) eval.	300-1000	$1.7 \times 10^{-13} \exp(-5000/T)$	b
	Westenberg, deHaas (1972a)	300	$\sim 1 \times 10^{-12}$	c,d
	Davis, Payne, Stief (1973)	300	$<10^{-20}$	e
	Wyrsch, et al (1974)	300	$<3 \times 10^{-18}$	
	Simonaitis, Heicklen (1973a)	373-473	$<5 \times 10^{-18}$	e
	Volman, Gorse (1972)	330	$<10^{-15}$	f
	Baldwin, Walker, Webster (1970)	713-773	$1 \times 10^{-10} \exp(-11500/T)$	e
	Vardanyan, Dangyan, Sachyan (1972)	878-952	$2.2 \times 10^{-10} \exp(-11500/T)$	

NOTE:
a. The low value of k selected in this evaluation is based on the evaluation by Lloyd and the measurements by Davis, Payne, Stief and Simonaitis, Heicklen.
b. Based on Davis, Payne and Stief (1972) and high T results. Temperature coef. probably maximum value.
c. Indirect measurement using a low-pressure discharge flow system.
d. Relative rate measurement - reference reaction: $H + HO_2 \rightarrow HO + HO$
e. Relative rate measurement - reference reaction: $HO_2 + HO_2 \rightarrow H_2O_2 + O_2$
f. Relative rate measurement - reference reaction: $HO + CO \rightarrow CO_2 + H$

20,48	$HO_2 + CH_2O \rightarrow H_2O_2 + CHO$			
	*Lloyd (1974) review	300-800	$1.7 \times 10^{-12} \exp(-4000/T)$	>±1 at 300K, ±0.2 at 800K
	Baldwin, et al (1972)	773	1.6×10^{-15}	(a)

(a) Derived by computer fit to data. Based on $k(HO_2 + HO_2 \rightarrow H_2O_2 + O_2) = 3.0 \times 10^{-12} cm^3 molecule^{-1} s^{-1}$

20,51	$HO_2 + CH_3O_2 \rightarrow CH_3O_2H + O_2$			
	Demerjian et al (1972) review	300	6.7×10^{-14}	estimate
20,57	$HO_2 + C_2H_4 \rightarrow C_2H_4O + HO$?			
	Walker (1973)	773	2.5×10^{-17}	(a)

(a) Relative to $k(HO_2 + HCHO) = 1.6 \times 10^{-15}$

20,57	$HO_2 + C_2H_4 \rightarrow$ addition products			
	Lloyd (1974) review	300	$\sim 1.7 \times 10^{-17}$	> ±1 (a)

(a) Suggestion. Data are irreconcilable.

20,58	$HO_2 + C_2H_6 \rightarrow H_2O_2 + C_2H_5$			
	Lloyd (1974) review	300-1000	$\sim 1.7 \times 10^{-12} \exp(-7000/T)$	±1 (a)

(a) Relative rate data versus $2HO_2 \rightarrow H_2O_2 + O_2$ and $HO_2 + CO \rightarrow HO + CO_2$. Temp. coef. estimated.

20,60	$HO_2 + C_3H_8 \rightarrow H_2O_2 + i\text{-}C_3H_7$			
	Lloyd (1974) review	300-1000	$<3.3 \times 10^{-13} \exp(-5300/T)$	±1 (a)

No.	Reaction/Reference * = Preferred Value + = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
			(a) Based on upper limit meas. Temp. coef. estimated.	
20,60	$H\dot{O}_2$ + $n\text{-}C_4H_{10}$ → H_2O_2 + $s\text{-}C_4H_9$ (primarily)			
	Lloyd (1974) review	300-1000	$8.3 \times 10^{-13} \exp(-5300/T)$	±1 (a)
	(a) Based on upper limit meas. Temp. coef. estimated.			
20,60	$H\dot{O}_2$ + $i\text{-}C_4H_{10}$ → H_2O_2 + $t\text{-}C_4H_9$			
	Lloyd (1974) review	300-1000	$1.7 \times 10^{-13} \exp(-3500/T)$	±1 (a)
	(a) Based on upper limit meas, Temp. coef. estimated.			
20,60	$H\dot{O}_2$ + alkane → H_2O_2 + alkyl radical			
	Walker (1977)	300-800	$k = 8 \times 10^{-14}[N_p \exp(-7520/T) + N_s \exp(-6330/T) + N_t \exp(-4990/T)]$ where N_p, N_s, and N_t are the number of primary, secondary, and tertiary hydrogen atoms respectively	
21,M	H_2 + M → H + H + M		see reverse reaction	
21,35	H_2 + Cl → HCl + H			
	+*Watson (1977) eval	200-300	$3.5 \times 10^{-11} \exp(-2290/T)$	±0.12 at 230K
	Watson, et al (1977)	213-350	$(5.5 \pm 0.5) \times 10^{-11} \exp(-2375 \pm 100/T)$	
	Lee, et al (1977)	200-500	$(2.66 \pm 0.42) \times 10^{-11} \exp(-2230 \pm 60/T)$	
21,36	H_2 + $Cl\dot{O}$ → products			
	+*NASA (1977) eval	200-300	$k \leq 1 \times 10^{-12} \exp(-4800/T)$	±2 at 230K (a)
	(a) "A factor" chosen. E_{act} fitted to upper limit at T = 670K reported in Watson's review (1977)			
22,29	$H_2\dot{O}$ + $S\dot{O}_3$ → products			
	Castleman, et al (1975)	298	$9.1 \pm 2.9 \times 10^{-13}$	
23,hν	H_2O_2 + hν → HO + HO			
	DeMore (1977)			

λ/nm	$10^{20} \times \sigma$	λ/nm	$10^{20} \times \sigma$ (a)
200	48.3	280	2.1
210	36.3	290	1.14
220	26.4	300	0.66
230	18.7	310	0.38
240	12.9	320	0.21
250	8.9	330	0.13
260	5.5	340	0.08
270	3.4	350	0.04

(a) σ is the absorption cross section in units of $cm^2 molecule^{-1}$ (base e). These values by DeMore (private communication) are in good agreement (within 10%) with unpublished results by Molina, et al and with results of Holt, et al (1948) over common ranges of measurements

	Hampson (1973) review		Quantum yields (primary) $\phi(-H_2O_2) = 1.0 \quad \lambda > 200nm$	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant k/cm^{3}molecule^{-1}s^{-1}	Notes and Reliability of log k
23,M	H_2O_2 + M → HO + HO + M		see reverse equation	
23,35	H_2O_2 + Cl → HCl + HO_2			
	†*Watson (1977) review	265-400	$1.7 \times 10^{-12}\exp(-384/T)$	±0.36 at 230K
23,35Br	H_2O_2 + Br → HBr + HO_2			
	†*NASA (1977) eval	200-300	$5 \times 10^{-12}\exp(-1570/T)$	±0.6 at 230K
24,M	HNO + M → H + NO + M			
	*Baulch, et al (1973) review	230-700	$5 \times 10^{-8}\exp(-24,500/T)$ M = H_2 (a) No data. Value based on reverse rate	±0.2 (a)
24,24	HNO + HNO → H_2O + N_2O			
	*Baulch, et al (1973) review	300	4×10^{-15}	±0.3
25,hν	HNO_2 + hν → HO + NO (a) → H + NO_2 (b)			
	Molina (1977) review	300	table of absorption cross sections for wavelength range 200-400nm. (a) Gives corrected values which supersede results in Johnston, Graham (1974). Also gives results of Cox and Derwent (1976)	(a)
	Cox, Derwent (1976)	300	table of absorption cross sections for λ = 200-400nm	
	Cox (1974b)		$\phi a \geq 0.97$ (a) Photolysis 330 < λ/nm < 380	(a)
26,hν	HNO_3 + hν → HO + NO_2		Elevation/km k(noon)/s^{-1} k(24 hr. av.)/s^{-1}	
	*Johnston (1974) review	217	15 5.1×10^{-7} 1.5×10^{-7}	±0.15
		217	20 7.7×10^{-7} 2.3×10^{-7}	Rates are for
		222	25 2.8×10^{-6} 6.8×10^{-7}	45° latitude
		227	30 1.4×10^{-5} 3.5×10^{-6}	solar equinox
		237	35 4.1×10^{-5} 1.2×10^{-5}	standard ozone
		251	40 7.6×10^{-5} 2.7×10^{-5}	background
		265	45 1.1×10^{-4} 4.2×10^{-5}	
	*Johnston, Graham (1973)		Table of absorption coefficients for λ = 190-325nm	
	Johnston, et al (1974)		ϕ = 1 200 < λ < 315nm (a) Products probably those shown above.	(a)
	Biaume (1973)		Absorption cross section data for for 185 < λ < 325 nm in good agreement with that of Johnston and Graham (1973).	
	Beddard, et al (1974)		figure showing extinction coefficient vs λ for λ = 120-170nm	
26,M	HNO_3 + M → HO + NO_2 + M		see reverse reaction	
26,35	HNO_3 + Cl → HCl + NO_3			
	†*NASA (1977) eval	200-300	$1.0 \times 10^{-11}\exp(-2170/T)$	±0.6 at 230K (a)
	Leu, DeMore (1976)	295	$(6.8 \pm 3.4) \times 10^{-15}$ (a) "A factor" chosen. E_{act} derived to fit room temp. result of Leu, DeMore.	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
26a,34b	$S + CS_2 \rightarrow S_2 + CS$			
	Baulch, et al (1976) review	298	6.5×10^{-13}	±0.2
26a,34c	$S + C\emptyset S \rightarrow C\emptyset + S_2$			
	Baulch, et al (1976) review	230-2600	$2.8 \times 10^{-12} \exp(-2050/T)$	±0.5
27,27	$S\emptyset + S\emptyset \rightarrow S\emptyset_2 + S$ or $(S\emptyset)_2$			
	Schofield (1973) review	300	$< 3 \times 10^{-15}$	
		1000	$< 2 \times 10^{-13}$	
	Chung, Calvert, Bottenheim (1975)	300	$8.3 \pm 6.7 \times 10^{-16}$	
27,29	$S\emptyset + S\emptyset_3 \rightarrow 2S\emptyset_2$			
	Chung, Calvert, Bottenheim (1975)	300	$2 \pm 1.2 \times 10^{-15}$	
28,49M	$S\emptyset_2 + CH_3 (+M) \rightarrow CH_3S\emptyset_2 (+M)$			
	James, et al (1973)	300	3×10^{-13} $cm^3 molecule^{-1} s^{-1}$	±0.1
31,31	$HS + HS \rightarrow H_2S + S$			
	Baulch, et al (1976) review	295	1.2×10^{-11}	±0.2
35,35M	$Cl + Cl + M \rightarrow Cl_2 + M$			
	*Watson (1977) review	200-500	$6 \times 10^{-34} \exp(900 \pm 250/T)$ $cm^6 molecule^{-2} s^{-1}$	M = Ar
35,37	$Cl + O\emptyset Cl \rightarrow 2Cl\emptyset$			
	†*Watson (1977) review	300-588	$(5.9 \pm 0.9) \times 10^{-11} \exp(0 \pm 120/T)$	±0.1
35,37	$Cl + Cl\emptyset\emptyset \rightarrow Cl_2 + \emptyset_2$ (a) $\rightarrow 2Cl\emptyset$ (b)			
	†*NASA (1977) eval		$k_a = 1.6 \times 10^{-10}$	
			$k_b = 1.1 \times 10^{-11}$	
	Johnston, et al (1969)	298	$k_a = 1.56 \times 10^{-10}$	
			$k_a/k_b = 108$	
	Nicholas, Norrish (1968)	298	$k_a/k_b = 15$	
35,44a	$Cl + Cl_2O \rightarrow Cl_2 + Cl\emptyset$			
	*Watson (1977) review	300	6.8×10^{-13}	
35,42	$Cl + N\emptyset Cl \rightarrow N\emptyset + Cl_2$			
	†*Watson (1977) review	298	$3 \pm 0.5 \times 10^{-11}$	
35,43	$Cl + N\emptyset_2Cl \rightarrow N\emptyset_2 + Cl_2$			
	Watson (1977) review	298	$k >> 3 \times 10^{-14}$	
35,43a	$Cl + N\emptyset_3Cl \rightarrow$ products			
	†*Kurylo, Manning (1977)	224-273	$1.68 \times 10^{-12} \exp(-607/T)$	±0.3
35,56	$Cl + CB_4 \rightarrow HCl + CH_3$			
	†*Watson (1977) review	200-300	$7.3 \times 10^{-12} \exp(-1269/T)$	(a)
	Manning, Kurylo (1977)	218-322	$(7.93 \pm 1.53) \times 10^{-12} \exp(-1273 \pm 51/T)$	
	Watson, et al (1976)	218-401	$(7.94 \pm 0.7) \times 10^{-12} \exp(-1260 \pm 35/T)$	(b)
	Whytock, et al (1977)	200-500	$5.44 \times 10^{-19} T^{2.50} \exp(-608/T)$	
		200-299	$(6.51 \pm 0.79) \times 10^{-12} \exp(-1229 \pm 27/T)$	
	Zahniser, et al (1978)	200-500	$8.6 \times 10^{-18} T^{2.11} \exp(-795/T)$	
		200-300	$(8.2 \pm 0.6) \times 10^{-12} \exp(-1320 \pm 20/T)$	
	Davis, et al (1970)	300	$1.5 \pm 0.1 \times 10^{-13}$	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
	Fettis, Knox (1964)		$4 \times 10^{-11} \exp(-1930/T)$	
	Clyne, Walker (1973)	300-686	$5.1 \times 10^{-11} \exp(-1790/T)$	
			(a) Based on four direct 1976, 1977 studies listed immediately below. Uncertainty in log k(230K) is +0.12 and -0.36	
			(b) Value changed subsequent to publication to allow for effect of small C_2H_6 impurity see Watson's review (1977)	
35,58	$Cl + C_2H_6 \rightarrow HCl + C_2H_5$			
	Manning, Kurylo (1977)	22-322	$(7.29 \pm 1.23) \times 10^{-11} \exp(-60 \pm 44/T)$	
36,hν	$ClO + h\nu \rightarrow Cl + O$			
	*Watson (1977) review		absorption cross section data $225 < \lambda < 300$ nm	
36,36	$ClO + ClO \rightarrow Cl + ClOO$ (a) $\rightarrow Cl_2 + O_2$ (b) $\rightarrow OClO + Cl$ (c)			
	†*NASA (1977) eval	200-300	$k_a = 1 \times 10^{-12} \exp(-1238/T)$	±0.2 at 230K (a)
			$k_b = 5 \times 10^{-13} \exp(-1238/T)$	±0.2 at 230K
			$k_c = 2 \times 10^{-12} \exp(-2200/T)$	±1 at 230K
			(a) $-d[ClO]/dt = k[ClO]^2$. Low pressure. See Watson's review (1977) for high pressure rec.	
36,36Br	$ClO + BrO \rightarrow Br + OClO$ (a) $\rightarrow Br + ClOO$ (b)			
	†*Watson (1977) review		$k_a = (6.7 \pm 1.0) \times 10^{-12}$	±0.36 at 230K
			$k_b = (6.7 \pm 1.0) \times 10^{-12}$	±0.36 at 230K
36,45	$ClO + CO \rightarrow CO_2 + Cl$			
	†*NASA (1977) eval	200-300	$k \leq 1 \times 10^{-12} \exp(-3700/T)$	±2 at 230K (a)
			(a) "A factor" chosen. E_{act} fitted to upper limit at T = 587K reported in Watson's review (1977)	
36,56	$ClO + CH_4 \rightarrow$ products			
	†*NASA (1977) eval	200-300	$k \leq 1 \times 10^{-12} \exp(-3700/T)$	±2 at 230K (a)
			(a) "A factor" chosen. E_{act} fitted to upper limit at T = 670K reported in Watson's review (1977)	
36,57	$ClO + C_2H_4 \rightarrow$ products			
	Walker (1972)	670	$k < 5 \times 10^{-16}$	(a)
			(a) As quoted by Watson (1977) review.	
36,59	$ClO + C_2H_2 \rightarrow$ products			
	Walker (1972)	670	$k < 5 \times 10^{-16}$	(a)
			(a) As quoted by Watson (1977) review.	
36Br,36Br	$BrO + BrO \rightarrow 2Br + O_2$			
	†*NASA (1977) eval	200-300	$2.9 \times 10^{-11} \exp(-450/T)$	±0.36 at 230K
	Clyne, Watson (1975)	298	6.4×10^{-12}	
	Clyne, Cruse (1970)	293	$5.3 \times 10^{-11} \exp(-450/T)$	

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
37,M	$ClOO + M \rightarrow Cl + O_2 + M$ Watson (1977) review			Table of values of rate constant as a function of altitude.
37,hν	$ClOO + h\nu \rightarrow ClO + O$ Watson (1977) review			absorption cross section data $225 < \lambda < 280$ nm
37,hν	$OClO + h\nu \rightarrow ClO + O$ Watson (1977) review			Abs. cross section data $150 < \lambda < 480$nm
39,hν	$HCl + h\nu \rightarrow H + Cl$ Watson (1977) review			absorption cross section data $140 < \lambda < 220$ nm
40,hν	$HOCl + h\nu \rightarrow$ products Watson (1977) review			Abs. cross section data $290 < \lambda < 450$nm
42,hν	$NOCl + h\nu$ Molina (1977) review			Table of absorption cross section values for λ = 190-400nm
43,hν	$ClNO_2 + h\nu$ Molina (1977) review			Absorption cross section data for λ = 190-400nm
43,hν	$ClONO + h\nu$ Molina (1977)			Absorption cross section data for λ = 235-400nm
43a,hν	$NO_3Cl + h\nu$ Rowland, Spencer, Molina (1976)			Table of absorption cross section values for λ = 186-460nm. Also table of solar photodissociation coefficients Data also tabulated in reviews by Watson (1977) and by Molina (1977). Molina's review also discusses quantum yield data
44,hν	$Cl_2 + h\nu \rightarrow 2Cl$ Watson (1977) review			absorption cross section data $240 < \lambda < 450$ nm
45,50	$CO + CH_3 \rightarrow . . .$			see $CH_3O + CO$
48,hν	$CH_2O + h\nu \rightarrow CH_2O^* \rightarrow H + HCO$ (1) $\rightarrow H_2 + CO$ (2) This survey (1978)			

λ/nm	Φ_1	$\Phi_1 + \Phi_2$
285	0.61	0.90
290	0.74	1
295	0.74	1
300	0.74	1
305	0.74	1
310	0.74	1
315	0.74	1
320	0.60	1
325	0.45	1
330	0.31	1

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k

335 0.17 1
340 0.02 0.64

Tentative recommendation based principally on results reported by Horowitz and Calvert (1978a) and by Moortgat, et al (1978). Also considers results reported in Clark, Moore and Nogar (1977), Horowitz and Calvert (1978b), Houston and Moore (1976), Lewis and Lee (1977), Lewis, Tang and Lee (1976) and Marling (1977).

Apparent quantum yield values are slightly higher in presence of O_2. Effect is assumed here to be due to secondary reactions.

Calvert, et al (1972)

λ/nm	10^{20} x σ	λ/nm	10^{20} x σ	(a)
290	3.18	330	2.36	
300	3.25	340	1.97	
310	3.14	350	0.84	
320	2.34	360	0.18	

(a) σ is the value of the absorption cross section averaged for 10nm bands. See McQuigg, Calvert (1969) for figure of of absn. coeff. vs wave length. Also see Miller and Lee (1977) for higher resolution spectra from which absorption cross section values can be derived.

50,4 $CH_3O + O_2 \rightarrow CH_2O + HO_2$ (1)

50,9 $CH_3O + NO \rightarrow CH_3ONO$ (2a)
$\rightarrow CH_2O + HNO$ (2b)

50,10 $CH_3O + NO_2 \rightarrow CH_3ONO_2$ (3a)
$\rightarrow CH_2O + HNO_2$ (3b)

50,45 $CH_3O + CO \rightarrow$ products (4)

*Heicklen (1973)

298 $k_1 \sim 3 \times 10^{-18}$
$\sim 1.6 \times 10^{-13} \exp(-3300/T)$
$k_2 \sim 8 \times 10^{-14}$

298 $k_1/k_2 = 4.7 \times 10^{-5}$ ±20% ratio probably is smaller at 220K

$k_{2b}/k_2 = 0.145$ ±0.015
$k_2/k_3 = 1.2$ ±0.1

298 $k_{2a}/k_{3a} = 1.1$
363 $= 1.8$
403 $= 2.7$

298 $k_{3a}/k_3 = 0.9$ ±0.1 k_{3a}/k_{3b} probably constant 300-400K

298 $k_{3b}/k_3 = 0.1$ ±0.01

298-423 $k_4/k_2 = 5 \times 10^{-4}$

Demerjian, et al (1974) review 300-400 $k_1 = 1.6 \times 10^{-17}$

No.	Reaction/Reference * = Preferred Value † = NASA (1977) eval	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
			$\sim 4.2 \times 10^{-13} \exp(-3000/T)$ adjusted to fit $C_4H_{10}/N\theta_x$ simulation studies $k_{2a} = 1.7 \times 10^{-13}$ $k_{2b}/k_{2a} = 0.17$ $k_{3a} = 3.3 \times 10^{-13}$ $k_{3b}/k_{3a} = 0.1$	
	Batt, McCulloch, Milne (1975)	393-473	$k_{2a} \sim 3 \times 10^{-11}$	±0.4
			$k_{2b} \sim 7 \times 10^{-12}$	±0.5
	Barker, et al (1977)	396-442	$k_1 = 5 \times 10^{-13} \exp(-2000/T)$	
51,51	$2CH_3\theta_2 \rightarrow 2CH_3\theta + \theta_2$ (a) $\rightarrow CH_3\theta H + CH_2\theta + \theta_2$ (b) $\rightarrow CH_3\theta_2CH_3 + \theta_2$ (c)			
	Weaver, et al (1975)	300	$k_a/k = 0.43$ $k_b/k = 0.50$ $k_c/k = 0.07$	
	Parkes (1977)	300	$k_a = 1.6 \pm 0.4 \times 10^{-13}$ $k_b + k_c = 3.0 \pm 0.8 \times 10^{-13}$	
54,hν	$CH_3\theta N\theta + h\nu \rightarrow CH_3\theta^* + N\theta$ (a) $\rightarrow$ isomer (b) $\rightarrow CH_2\theta + HN\theta$ (c) $\rightarrow CH_2\theta + H + N\theta$ (d)			
	*Heicklen (1973) review	298	$k_a/k = 0.76 \pm 0.02$, $\lambda = 366nm$	
		298	$k_b/k = 0.24 \pm 0.04$, $\lambda = 366nm$	
		298	$(k_c + k_d)/k < 0.02$, $\lambda = 366nm$ $k = k_a + k_b + k_c + k_d$	
61,hν	$CF_2Cl_2 + h\nu$			
	Watson (1977) review		Absorption cross section data for $174 < \lambda/nm < 220$	
	Molina (1977) review		Low temperature absorption cross section data	
62,hν	$CFCl_3 + h\nu$			
	Watson (1977) review		Tabulated values of absorption cross sections for $174 < \lambda/nm < 230$.	
	Molina (1977) review		Low temperature abs. cross section data	
63,hν	$CCl_4 + h\nu$			
	Watson (1977) review		Absorption cross section data for $174 < \lambda/nm < 238$. see Watson's review (1977)	

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APPENDIX 1.

Chemical Thermodynamic Properties of Selected Molecular Species

E. S. Domalski, D. Garvin, and D. D. Wagman

Two tables are provided showing chemical thermodynamic properties of selected molecular species of interest in stratospheric chemistry. In these tables there are sufficient data for the usual calculations of heats of reaction and equilibria.

The first table lists enthalpy and Gibbs energy of formation, entropy and heat capacity data. The information was extracted from "Selected Values of Chemical Thermodynamic Properties" (D. D. Wagman, et al, NBS Technical Note 270-3, January 1968) except as indicated in the Notes. The thermodynamic properties tabluated are:

1. enthalpy of formation at OK and 298.15K,
2. Gibbs energy of formation at 298.15K,
3. enthalpy increment between OK and 298.15K,
4. entropy at 298.15K,
5. heat capacity at constant pressure at 298.15K.

The values given for the heats of formation are based on experimental thermodynamic and spectroscopic measurements except where otherwise indicated; the values of $S°$, $C_p°$ and $H°_{298}-H°_0$ for gaseous species were calculated by standard statistical-mechanical equations, using corrections for vibrational anharmonicities, rotational stretching, and rotation-vibration interactions where these data were available.

The second table presents bond dissociation energies or bond strengths. These usually are the enthalpies of simple bond scission reactions. However, there are some cases in which there is a substantial contribution from rearrangement of electronic structure in the products (reducing the bond energy).

The values given here for some molecules may differ slightly from values adopted by the CODATA Task Group on Key Values for Thermodynamics (see CODATA Bulletin 17, published by the International Council of Scientific Unions Committee on Data for Science and Technology, January 1976). These differences will have no significant effect on the enthalpies or free energies of reaction calculated from the tables.

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity *

Substance			ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°	
Formula and Description	State	Formula Weight	0 °K	298.15 °K (25 °C)					
			kcal/mol				cal/deg mol		
O oxygen, atomic	g	15.9994	58.983	59.553	55.389	1.607	38.467	5.237	
$O(^1D)$	g	15.9994	104.34	104.78		1.481			(1)
$O(^1S)$	g	15.9994	155.60	156.04		1.481			(1)
O_2 oxygen, molecular, $(^3\Sigma_g^-)$	g	31.9988	0	0	0	2.0746	49.003	7.016	(2)
$O_2(^1\Delta)$	g	31.9988	22.54	22.54					(1)
$O_2(^1\Sigma)$	g	31.9988	37.51	37.51					(1)
O_3 ozone	g	47.9982	34.74	34.1	39.0	2.4736	57.08	9.37	
H hydrogen, atomic	g	1.0080	51.633	52.103	48.588	1.481	27.391	4.9679	(30)
H_2 hydrogen, molecular	g	2.0159	0	0	0	2.0238	31.208	6.889	
OH hydroxyl	g	17.0074	9.25	9.31	8.18	2.1070	43.890	7.143	
HO_2 hydroperoxyl	g	33.0068	1.2±2	0.5±2	3.4	2.39	54.73	8.34	(34)
H_2O water	g	18.0153	-57.102	-57.796	-54.634	2.3667	45.104	8.025	
H_2O_2 hydrogen peroxide	g	34.0147	-31.08	-32.58	-25.24	2.594	55.6	10.3	
N nitrogen, atomic	g	14.0067	112.534	112.979	108.883	1.481	36.622	4.968	
N_2 nitrogen, molecular	g	28.0134	0	0	0	2.072	45.77	6.961	
NO nitric oxide	g	30.0061	21.45	21.57	20.69	2.197	50.347	7.133	
NO_2 nitrogen dioxide	g	46.0055	8.60	7.93	12.26	2.438	57.35	8.89	
NO_3 nitrogen trioxide	g	62.008	18.5	17.0	27.7	2.62	60.4	11.2	(3)
N_2O nitrous oxide	g	44.0128	20.435	19.61	24.90	2.284	52.52	9.19	
N_2O_4 dinitrogen tetroxide	g	92.0110	4.49	2.19	23.38	3.918	72.70	18.47	

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Substance			ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°	
Formula and Description	State	Formula Weight	0 °K	298.15 °K (25 °C)					
			kcal/mol				cal/deg mol		
N_2O_5 dinitrogen pentoxide	g	108.0104	5.7	2.7	27.5	4.237	85.0	20.2	
NH imino (imidogen)	g	15.0147	82.	82.	80.6	2.060	43.29	6.97	(29)
NH_2 amino	g	16.0226	46.2	45.5	47.8	2.37	46.51	8.02	(4)
NH_3 ammonia	g	17.0306	-9.31	-10.98	-3.93	2.40	46.05	8.38	(30)
HNO nitroxyl hydride	g	31.0142	24.5	23.8	26.859	2.387	52.729	8.279	(3)
HNO_2 cis, nitrous acid	g	47.0135	-17.12	-18.64	-10.27	2.608	59.43	10.70	
trans, nitrous acid	g	47.0135	-17.68	-19.15	-10.82	2.652	59.54	11.01	
cis-trans mixture, equil.	g	47.0135		-19.0	-11.0		60.7	10.9	
HNO_3 nitric acid	g	63.0129	-29.94	-32.28	-17.87	2.815	63.64	12.75	
S sulfur, rhombic	c	32.064	0	0	0	1.054	7.60	5.41	
	g	32.064	65.7	66.20	56.52	1.591	40.085	5.658	(30)
SO monosulfur monoxide	g	48.0634	1.2	1.2	-5.0	2.087	53.02	7.21	(32)
SO_2 sulfur dioxide	g	64.0628	-70.33	-70.94	-71.74	2.521	59.30	9.53	(30)
SO_3 sulfur trioxide	c	80.0622		-108.63	-88.19		12.5		
	liq	80.0622		-105.41	-88.04		22.85		
	g	80.0622	-93.21	-94.58	-88.69	2.796	61.34	12.11	
H_2SO_4 sulfuric acid	c	98.0775	-194.069						
	liq	98.0775		-194.548	-164.938	6.748	37.501	33.20	
S_2O disulfur monoxide	g	80.1274				2.66	63.8	10.5	(3)
HS sulfur monohydride	g	33.0720	33.1	33.3	26.3	2.22	46.73	7.76	(5)

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Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Substance			ΔHf_0°	ΔHf°	ΔGf°	$H_{298}^\circ - H_0^\circ$	S°	C_p°	
Formula and Description	State	Formula Weight	0°K	298.15°K (25°C)					
			kcal/mol				cal/deg mol		
H_2S hydrogen sulfide	g	34.0799	-4.232	-4.93	-8.02	2.379	49.16	8.18	
C graphite, Acheson spectroscopic	c	12.0112	0	0	0	0.251	1.372	2.038	
CO carbon monoxide	g	28.0106	-27.199	-26.416	-32.780	2.0716	47.219	6.959	
CO_2 carbon dioxide	g	44.0100	-93.963	-94.051	-94.254	2.2378	51.06	8.87	
CH_3 methyl	g	15.0351	35.6	34.8	35.3	2.49	46.38	9.25	(3)
CH_4 methane	g	16.0430	-15.970	-17.88	-12.13	2.388	44.492	8.439	
HCO formyl	g	29.0185	8.9	9.0	5.36	2.386	53.68	8.26	(8)
HCHO formaldehyde	g	30.0265	-25.03	-25.95	-24.51	2.394	52.26	8.46	(6)
CH_3O methoxy	g	31.0345	5.8	3.9	6.4	2.41	64.2	8.9	(7) (24)
CH_3O_2 methylperoxyl	g	47.0339		6.7					(8)
CH_3OOH methyl hydroperoxide	g	48.0347		-30.8	-17.4		67.9	15.	(9)
CH_3NO_2 nitromethane	g	61.0406	-14.546	-17.86	-1.65	3.083	65.69	13.70	
CH_3ONO methyl nitrite	g	61.0406	-13.5	-16.5	-1.5	3.36	69.7	16.5	(10)(24)
CH_3NO_3 methyl nitrate	g	77.0400	-25.9	-29.8	-9.4	3.55	76.1	16.1	(11, 12)(24)
$COCl_2$ phosgene	g	98.9166	-52.195	-52.61	-49.20	3.067	67.74	13.78	(13)

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Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table

Substance			ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°	
Formula and Description	State	Formula Weight	0 °K	298.15 °K (25 °C)					
			kcal/mol				cal/deg mol		
C_2H_2 acetylene	g	26.0382	54.324	54.19	50.00	2.392	48.00	10.50	
C_2H_4 ethylene	g	28.0542	14.515	12.49	16.28	2.525	52.45	10.41	
C_2H_5 ethyl radical	g	29.0627		25.7	32.0		59.6	10.9	(14)
C_2H_6 ethane	g	30.0701	-16.323	-20.04	-7.66	2.856	54.85	12.58	(15,16)
C_3H_6 propylene	g	42.0816	8.467	4.88	15.00	3.237	63.80	15.27	(15)
C_3H_8 propane	g	44.0976	-19.684	-25.02	-5.81	3.512	64.51	17.57	(15,16)
C_4H_{10} n-butane	g	58.1248	-23.552	-30.03	-3.97	4.645	74.12	23.29	(15,16)
C_4H_{10} isobutane	g	58.1248	-25.223	-32.07	-4.91	4.276	70.42	23.14	(15,16)
CH_2CO ketene	g	42.0376	-10.66	-11.4	-11.6	2.819	59.16	12.37	(17)
CH_3CO acetyl radical	g	43.0456		-5.8	-3.0		64.5	12.7	(19)
CH_3CHO acetaldehyde	g	44.0536	-37.14	-39.72	-30.31	3.01	59.8	13.7	
CH_3COCl acetyl chloride	g	78.4986	-57.93	-60.07	-51.08	3.529	70.56	16.25	(18)
Cl chlorine, atomic	g	35.453	28.59	28.992	25.173	1.499	39.457	5.220	(30)
ClO chlorine monoxide	g	51.4524	24.33	24.47	23.68	2.278	53.78	8.23	(20)
ClO_2 chlorine dioxide (sym.)	g	67.4518	25.09	24.5	28.8	2.580	61.36	10.03	

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Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table

Substance			ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°	
Formula and Description	State	Formula Weight	0 °K	298.15 °K (25 °C)					
			kcal/mol				cal/deg mol		
ClO_2 chlorine dioxide (unsym.)	g	67.4518	21.7	21.3	25.1	2.78	63.0	11.0	(21)
ClO_3 chlorine trioxide	g	83.4512		37					
HCl hydrogen chloride	g	36.4610	-22.020	-22.062	-22.777	2.066	44.646	6.96	
HOCl hypochlorous acid	g	52.4604	-18.0	-18.7	-15.7	2.440	56.54	8.88	(31)
NOCl nitrosyl chloride	g	65.4591	12.81	12.36	15.77	2.716	62.52	10.68	
NO_2Cl nitryl chloride	g	81.4585	4.29	3.0	13.0	2.915	65.02	12.71	
NO_3Cl chlorine nitrate	g	97.458		6.28					(33)
Cl_2 chlorine, molecular	g	70.906	0	0	0	2.193	53.288	8.104	
Cl_2O dichlorine monoxide	g	86.9054	19.62	19.20	23.3	2.806	64.07	11.48	(22)
Cl_2O_4 chlorine perchlorate	g	134.9036				4.16	78.21	20.56	(23)
CF_4 carbon tetrafluoride	g	88.0048	-221.61	-223.04	-212.37	3.043	62.45	14.59	(3)
$CClF_3$ chlorotrifluoromethane	g	104.4594	-168.0	-169.2	-159.5	3.294	68.17	15.99	(3)
CF_2Cl_2 dichlorodifluoromethane	g	120.9140	-116.5	-117.5	-108.2	3.553	71.91	17.31	(3)
CCl_3F trichlorofluoromethane	g	137.3686	-68.24	-69.0	-59.6	3.838	74.00	18.65	(3)
CCl_4 carbon tetrachloride	g	153.8232	-22.42	-22.94	-12.83	4.120	74.02	19.93	(3, 25, 26)

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Table

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Substance			ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C_p°	
Formula and Description	State	Formula Weight	0°K	298.15°K (25°C)					
			kcal/mol				cal/deg mol		
CH_3Cl methyl chloride	g	50.4881	-17.69	-19.59	-13.98	2.489	55.99	9.73	(3, 27)
CH_2Cl_2 methylene dichloride	g	84.9331	-21.19	-22.83	-16.49	2.830	64.57	12.16	(3, 25)
$CHCl_3$ chloroform	g	119.3781	-23.49	-24.66	-16.83	3.383	70.63	15.63	(3, 25)
CF_3 trifluoromethyl radical	g	69.0064	-111.7	-112.4	-109.21	2.754	63.33	11.90	(3)
CCl_3 trichloromethyl radical	g	118.3702	19.15	19.	22.09	3.392	70.92	15.21	(3)
C_2Cl_4 tetrachloroethylene	g	165.8343	-2.83	-2.97	5.15	4.759	82.05	22.84	(3)
C_2HCl_3 trichloroethylene	g	131.3893	-1.032	-1.86	4.31	3.975	77.6	19.18	
CH_3CCl_3 1,1,1-trichloroethane (methyl chloroform)	g	133.4052	-34.65	-34.01	-18.21	4.30	76.49	22.07	(28)

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Notes

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2. Contributions of the higher electronic states of molecular oxygen to the enthalpy, entropy, and heat capacity at 298 K are insignificant.

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9. Values for $\Delta Hf°$, $S°$, and $Cp°$ at 298.15 K were calculated using the group additivity method described by Benson and O'Neal ("Kinetic Data on Gas Phase Unimolecular Reactions", NSRDS-NBS-21, Feb. 1970, pp. 40-42).

10. The value for ΔHf° [$CH_3ONO(g)$] = -16.5 kcal mol^{-1} was derived from the combustion data of Geiseler and Thierfelder (Z. physik. Chem., N. F., 29, 248-257 (1961)), and the equilibrium data of Leermakers and Ramsperger (J. Am. Chem. Soc. 54, 1837-1845 (1932)) for: $CH_3OH(g) + NOCl(g) = CH_3ONO(g) + HCl(g)$.

11. The value for ΔHf° ($CH_3ONO_2(g)$) = -29.8 kcal mol^{-1} was derived from the work of Ray and Ogg (J. Phys. Chem. 63, 1522-1523 (1959)) on the enthalpy of reaction of N_2O_5 with CH_3ONO.

12. We have chosen S° [$CH_3ONO_2(g)$] = 76.1 cal $mol^{-1}K^{-1}$ based upon low temperature thermal data of Gray and Smith (J. Chem. Soc. 1953, 2380-2385). Calculations from microwave studies by Dixon and Wilson (J. Chem. Phys. 35, 191-198 (1961)) give S° = 72.15 cal $mol^{-1}K^{-1}$.

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Bond Dissociation Energies, D_o^o at 0 K

Calculated from heats of formation in the accompanying table

Reaction	kJ/mol	kcal/mol	Note
$O_2 \rightarrow 2O$	493.59±0.4	117.97±0.1	
$O_3 \rightarrow O_2 + O$	101.4±2.1	24.24±0.5	
$H_2 \rightarrow 2H$	432.00±0.04	103.25±0.01	
$HO \rightarrow H + O$	423.8±2.1	101.3±0.5	
$HO_2 \rightarrow HO + O$	280±8	67±2	
$\rightarrow H + O_2$	210±8	50±2	
$H_2O \rightarrow HO + H$	493.7±0.8	118.0±0.2	
$H_2O_2 \rightarrow 2HO$	207.1±2.1	49.5±0.5	
$H_2O_2 \rightarrow H + HO_2$	350±8	84±2	
$N_2 \rightarrow N + N$	941.69±0.04	225.07±0.01	
$NO \rightarrow N + O$	627.9	150.1	
$NO_2 \rightarrow NO + O$	300.5	71.83	
$NO_3 \rightarrow NO_2 + O$	205±21	49±5	
$N_2O \rightarrow N + NO$	474.9±4	113.5±1	
$\rightarrow N_2 + O$	161.3	38.58	
$N_2O_3 \rightarrow NO + NO_2$	35.1±0.8	8.4±0.2	
$N_2O_4 \rightarrow NO_2 + NO_2$	53.2	12.7	
$N_2O_5 \rightarrow NO_2 + NO_3$	89.5	21.4	
$HNO \rightarrow H + NO$	203	48.6	
$\rightarrow NH + O$	487	116.5	
trans-$HNO_2 \rightarrow HO + NO$	202	48.4	
$HNO_3 \rightarrow HO + NO_2$	200	47.8	
$NH \rightarrow H + N$	343	82	

Bond Dissociation Energies, D_o^o at 0 K

Calculated from heats of formation in the accompanying table

Reaction	kJ/mol	kcal/mol	Note
$NH_2 \rightarrow H + HN$	366	87.4	
$NH_3 \rightarrow NH_2 + H$	448	107	
$CO \rightarrow C + O$	1071.94±0.4	256.2±0.1	
$CO_2 \rightarrow CO + O$	525.9±0.4	125.7±0.1	
$CHO \rightarrow CO + H$	70	16.7	(1)
$CH_2O \rightarrow CHO + H$	364	87	(1)
$CH_3O \rightarrow CH_3 + O$	378	90.4	(1)
$\rightarrow H + H_2CO$	93	22	(1)
$CH_3O_2 \rightarrow CH_3O + O$	237	56.8	(1)
$\rightarrow CH_3 + O_2$	118	28.1	(1)
$CH_4 \rightarrow CH_3 + H$	432	103.2	
$CH_3OOH \rightarrow CH_3O + HO$	184.	44.0	(1)
$\rightarrow CH_3 + HO_2$	276±8	66±2	(1)
$CH_3ONO \rightarrow CH_3 + NO_2$	248	59.2	(1)
$CH_3NO_2 \rightarrow CH_3 + NO_2$	254	60.6	(1)
$CH_3ONO_2 \rightarrow CH_3O + NO_2$	174	41.6	(1)
$\rightarrow CH_3 + NO_3$	341	81.6	(1)
$SO \rightarrow S + O$	515.4±8	123.2±2	
$SO_2 \rightarrow SO + O$	547.3±8	130.8±2.0	
$SO_3 \rightarrow SO_2 + O$	342.7±4	81.9±1	

Note 1. Calculated for T = 298K

APPENDIX 2. CONVERSION TABLES

EQUIVALENT SECOND ORDER RATE CONSTANTS

A \ B	$cm^3 mol^{-1} s^{-1}$	$dm^3 mol^{-1} s^{-1}$	$m^3 mol^{-1} s^{-1}$	$cm^3 molecule^{-1} s^{-1}$	$(mm\ Hg)^{-1} s^{-1}$	$atm^{-1} s^{-1}$	$ppm^{-1} min^{-1}$	$m^2 kN^{-1} s^{-1}$
1 $cm^3 mol^{-1} s^{-1}$ =	1	10^{-3}	10^{-6}	1.66×10^{-24}	$1.604 \times 10^{-5} T^{-1}$	$1.219 \times 10^{-2} T^{-1}$	2.453×10^{-9}	$1.203 \times 10^{-4} T^{-1}$
1 $dm^3 mol^{-1} s^{-1}$ =	10^3	1	10^{-3}	1.66×10^{-21}	$1.604 \times 10^{-2} T^{-1}$	$12.19\ T^{-1}$	2.453×10^{-6}	$1.203 \times 10^{-1} T^{-1}$
1 $m^3 mol^{-1} s^{-1}$ =	10^6	10^3	1	1.66×10^{-18}	$16.04\ T^{-1}$	$1.219 \times 10^4 T^{-1}$	2.453×10^{-3}	$120.3\ T^{-1}$
1 $cm^3 molecule^{-1} s^{-1}$ =	6.023×10^{23}	6.023×10^{20}	6.023×10^{17}	1	$9.658 \times 10^{18} T^{-1}$	$7.34 \times 10^{21} T^{-1}$	1.478×10^{15}	$7.244 \times 10^{19} T^{-1}$
1 $(mm\ Hg)^{-1} s^{-1}$ =	$6.236 \times 10^4 T$	$62.36\ T$	$6.236 \times 10^{-2} T$	$1.035 \times 10^{-19} T$	1	760	4.56×10^{-2}	7.500
1 $atm^{-1} s^{-1}$ =	$82.06\ T$	$8.206 \times 10^{-2} T$	$8.206 \times 10^{-5} T$	$1.362 \times 10^{-22} T$	1.316×10^{-3}	1	6×10^{-5}	9.869×10^{-3}
1 $ppm^{-1} min^{-1}$ = at 298K, 1 atm. total pressure	4.077×10^8	4.077×10^5	407.7	6.76×10^{-16}	21.93	1.667×10^4	1	164.5
1 $m^2 kN^{-1} s^{-1}$ =	$8314\ T$	$8.314\ T$	$8.314 \times 10^{-3} T$	$1.38 \times 10^{-20} T$	0.1333	101.325	6.079×10^{-3}	1

To convert a rate constant from one set of units A to a new set B find the conversion factor for the row A under Column B and multiply the old value by it, e.g. to convert $cm^3 molecule^{-1} s^{-1}$ to $m^3 mol^{-1} s^{-1}$ multiply by 6.023×10^{17}.

Table adapted from Evaluated Kinetic Data for High Temperature Reactions, Volume 1: Homogeneous Gas Phase Reactions of the H_2-O_2 System, Butterworths, London, 1972.

EQUIVALENT THIRD ORDER RATE CONSTANTS

A \ B	$cm^6 mol^{-2} s^{-1}$	$dm^6 mol^{-2} s^{-1}$	$m^6 mol^{-2} s^{-1}$	$cm^6 molecule^{-2} s^{-1}$	$(mm\ Hg)^{-2} s^{-1}$	$atm^{-2} s^{-1}$	$ppm^{-2} min^{-1}$	$m^4 kN^{-2} s^{-1}$
1 $cm^6 mol^{-2} s^{-1}$ =	1	10^{-6}	10^{-12}	2.76×10^{-48}	$2.57 \times 10^{-10} T^{-2}$	$1.48 \times 10^{-4} T^{-2}$	1.003×10^{-19}	$1.447 \times 10^{-8} T^{-2}$
1 $dm^6 mol^{-2} s^{-1}$ =	10^6	1	10^{-6}	2.76×10^{-42}	$2.57 \times 10^{-4} T^{-2}$	$148\ T^{-2}$	1.003×10^{-13}	$1.447 \times 10^{-2} T^{-2}$
1 $m^6 mol^{-2} s^{-1}$ =	10^{12}	10^6	1	2.76×10^{-36}	$257\ T^{-2}$	$1.48 \times 10^{8} T^{-2}$	1.003×10^{-7}	$1.447 \times 10^{4} T^{-2}$
1 $cm^6 molecule^{-2} s^{-1}$ =	3.628×10^{47}	3.628×10^{41}	3.628×10^{35}	1	$9.328 \times 10^{37} T^{-2}$	$5.388 \times 10^{43} T^{-2}$	3.64×10^{28}	$5.248 \times 10^{39} T^{-2}$
1 $(mm\ Hg)^{-2} s^{-1}$ =	$3.89 \times 10^{9} T^2$	$3.89 \times 10^{3} T^2$	$3.89 \times 10^{-3} T^2$	$1.07 \times 10^{-38} T^2$	1	5.776×10^{5}	3.46×10^{-5}	56.25
1 $atm^{-2} s^{-1}$ =	$6.733 \times 10^{3} T^2$	$6.733 \times 10^{-3} T^2$	$6.733 \times 10^{-9} T^2$	$1.86 \times 10^{-44} T^2$	1.73×10^{-6}	1	6×10^{-11}	9.74×10^{-5}
1 $ppm^{-2} min^{-1}$ = at 298K, 1 atm. total pressure	9.97×10^{18}	9.97×10^{12}	9.97×10^{6}	2.75×10^{-29}	2.89×10^{4}	1.667×10^{10}	1	1.623×10^{6}
1 $m^4 kN^{-2} s^{-1}$ =	$6.91 \times 10^{7} T^2$	$69.1\ T^2$	$6.91 \times 10^{-5} T^2$	$1.904 \times 10^{-40} T^2$	0.0178	1.027×10^{4}	6.16×10^{-7}	1

See note to Table for Second Order Rate Constants

CONVERSION FACTORS FOR UNITS OF OPTICAL ABSORPTION COEFFICIENTS

A \ B	(cross section σ) cm^2 molecule^{-1} base e	(atm at 273)$^{-1}$ cm^{-1} base e	dm^3 mol^{-1} cm^{-1} base 10	cm^2 mol^{-1} base 10
1 (atm at 298)$^{-1}$ cm^{-1} base e =	4.06×10^{-20}	1.09	10.6	1.06×10^{4}
1 (atm at 298)$^{-1}$ cm^{-1} base 10 =	9.35×10^{-20}	2.51	24.4	2.44×10^{4}
1 (mm Hg at 298)$^{-1}$ cm^{-1} base 10 =	7.11×10^{-17}	1.91×10^{3}	1.86×10^{4}	1.86×10^{7}
1 (atm at 273)$^{-1}$ cm^{-1} base e =	3.72×10^{-20}	1	9.73	9.73×10^{3}
1 (atm at 273)$^{-1}$ cm^{-1} base 10 =	8.57×10^{-20}	2.303	22.4	2.24×10^{4}
1 dm^3 mol^{-1} cm^{-1} base 10 =	3.82×10^{-21}	0.103	1	10^{3}
1 cm^2 mol^{-1} base 10 =	3.82×10^{-24}	1.03×10^{-4}	10^{-3}	1
1 cm^2 molecule^{-1} base e =	1	2.69×10^{19}	2.62×10^{20}	2.62×10^{23}

To convert an absorption coefficient from one set of units A to a new set B, multiply by the value tabulated for row A under column B, e.g. to convert the value of the absorption coefficient expressed in dm^3 mol^{-1} cm^{-1} base 10 to (atm at 273)$^{-1}$ cm^{-1} base e, multiply by 0.103.

NBS-114A (REV. 7-73)

U.S. DEPT. OF COMM. BIBLIOGRAPHIC DATA SHEET	1. PUBLICATION OR REPORT NO. NBS SP-513	2. Gov't Accession No.	3. Recipient's Accession No.

4. TITLE AND SUBTITLE

Reaction Rate and Photochemical Data for Atmospheric Chemistry - 1977

5. Publication Date: May 1978

6. Performing Organization Code

7. AUTHOR(S)

Robert F. Hampson, Jr., and David Garvin, Editors

8. Performing Organ. Report No.

9. PERFORMING ORGANIZATION NAME AND ADDRESS

NATIONAL BUREAU OF STANDARDS
DEPARTMENT OF COMMERCE
WASHINGTON, D.C. 20234

10. Project/Task/Work Unit No.

11. Contract/Grant No.

12. Sponsoring Organization Name and Complete Address *(Street, City, State, ZIP)*

Department of Transportation, FAA, Washington, DC 20591
N.A.S.A., Washington, DC 20546
Office of Standard Reference Data, NBS, Washington, DC 20234
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13. Type of Report & Period Covered

14. Sponsoring Agency Code

15. SUPPLEMENTARY NOTES

Library of Congress Catalog Card Number: 78-606033

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A table of data for gas phase chemical reactions and photochemistry of neutral species is presented. Specifically, it gives preferred values for reaction rate constants, photoabsorption cross sections, and quantum yields of primary photochemical processes and also cites recent experimental work (to December 1977). It is intended to provide the basic physical chemical data needed as input data for calculations modelling atmospheric chemistry. An auxiliary table of thermochemical data for the pertinent chemical species is given in the appendix.

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UNCLASSIFIED	111
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USCOMM-DC 29042-P74

☆ U. S. GOVERNMENT PRINTING OFFICE : 1978 261-238/88

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